SPECTRAL ANALYSIS OF METRIC GRAPHS AND RELATED SPACES

OLAF POST

Abstract. The aim of the present article is to give an overview of spectral theory on metric graphs guided by spectral geometry on discrete graphs and manifolds. We present the basic concept of metric graphs and natural Laplacians acting on it and explicitly allow infinite graphs. Motivated by the general form 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. Moreover, we describe a connection of metric graphs with manifolds. Finally, we comment on Cheeger's inequality and trace formulas for metric and discrete (generalised) Laplacians.

1. Introduction

A *metric graph* X 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 are playing 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 Section 5. On the other hand, solving a system of ODEs reduces in many cases to a discrete problem on the combinatorial graph, see Section 4.

The spectral relation between metric and (generalised) discrete Laplacians has the simplest form if the graph is *equilateral*, i.e., if all lengths are the same, say, $\ell_e = 1$. This fact and related results have already been observed by many authors (see e.g. [vB85, C97, CaW05, Pa06, BaF06, Pa07, P07a, BGP08] and the references therein). Moreover, for non-equilateral graphs, one has at least a spectral relation at the bottom of the spectrum. In particular, one can define an *index* (the Fredholm index of a generalised "exterior derivative" in the discrete and metric case) and show that they agree (Theorem 4.3). 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 [KPS07, FKW07, P07b]. For convergence results of a sequence of discrete Laplacians towards a metric graph Laplacian, we refer to [F06] and the references therein.

Spectral graph theory is an active area of research. We do not attempt to give a complete overview here, and the choice of the selected topics depends much on the author's taste. Results on spectral theory of combinatorial Laplacians can be found e.g. in [D84, MW89, CdV98, CGY96, Ch97, HSh99, Sh00, HSh04]. For metric graph Laplacians we mention the works [R84, vB85, N87, KoS99, Ha00, KoS03, K04, FT04a, K05, BaF06, KoS06, Pa06, HP06, BaR07].

Many concepts from spectral geometry on manifolds carry over to metric and discrete graphs, and the right notion for a general scheme would be a metric measure space with a Dirichlet form. In particular, metric graphs fall into this class; and they can serve as a toy model in order to provide new results in spectral geometry.

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 describe relations between the discrete and metric graph Laplacians. Section 5 contains the relation of a metric graph with a family of manifolds converging to it. Section 6 is devoted to the study of the first

Date: February 15, 2008, *File:* lausanne-proc.tex.

non-zero eigenvalue of the Laplacian. In particular, we show Cheeger's inequality for the (standard) metric graph Laplacian. Section 7 contains material on trace formulas for the heat operator associated to (general) metric and discrete graph Laplacians. In particular, we show a "discrete path integral" formula for generalised discrete graph Laplacians (cf. Theorem 7.7).

Outlook and further developments. Let us mention a few aspects which are not included in this article in order to keep it at a reasonable size. Our basic assumption is a lower bound on the edge lengths. If we drop this condition, we obtain *fractal* metric graphs, i.e., (infinite) metric graphs with $\inf_e \ell_e = 0$. A simple example is given by a rooted tree, where the length ℓ_n of an edge in generation n tends to 0. New effects occur in this situation: for example, the Laplacian on compactly supported functions can have more than one self-adjoint extension; one needs additional boundary conditions at infinity (see e.g. [So04]).

Another interesting subject are (infinite) covering graphs with finite or compact quotient, for example Cayley graphs associated to a finitely generated group. For example, if the covering group is Abelian, one can reduce the spectral theory to a family of problems on the quotient (with discrete spectrum) using the so-called *Floquet* theory. There are still open questions, for example whether the (standard) discrete Laplacian of an equilateral maximal Abelian covering has full spectrum or not. This statement is proven if all vertices have even degree (using an "Euler"-circuit). One can ask whether similar statements hold also for general metric graph Laplacians. For more details, we refer to [HSh99] and the references therein.

Metric graphs have a further justification: The wave equation associated to the (standard) metric graph Laplacian has finite propagation speed, in contrast to the corresponding equation for the (standard) discrete Laplacian (see [FT04b, Sec. 4] for details). Note that the latter operator is bounded, whereas the metric graph Laplacian is unbounded as differential operator. Therefore, one can perform wave equation techniques on metric graphs (and indeed, this has been done, see for example the scattering approach in [KoS99]).

Acknowledgements. The author would like to thank the organisers of the programme "Limits of graphs in group theory and computer science" held at the Bernoulli Center of the *École Polytechnique Fédérale de Lausanne* (EPFL), especially Prof. Alain Valette, for the kind invitation and hospitality. The present article is an extended version of a lecture held at the EPFL in March 2007.

2. Discrete graphs and general Laplacians

In this section, we define a generalised discrete Laplacian, which occurs also in the study of metric graph Laplacians as we will see in Section 4.

Let us fix the notation: Suppose G is a countable, discrete, weighted graph given by (V, E, ∂, ℓ) where (V, E, ∂) is a usual graph, i.e., V denotes the set of vertices, E denotes the set of edges, $\partial\colon E \longrightarrow V \times V$ associates to each edge e the pair $(\partial_- e, \partial_+ e)$ of its initial and terminal point (and therefore an orientation). Abusing the notation, we also denote by ∂e the *set* $\{\partial_- e, \partial_+ e\}$.

That G is an *(edge-)weighted* graph means that there is a *length* or *(inverse) edge weight function* $\ell\colon E \longrightarrow (0, \infty)$ associating to each edge e a length ℓ_e. For simplicity, we consider *internal* edges only, i.e., edges of *finite* length $\ell_e < \infty$, and we also make the following assumption on the lower bound of the edge lengths:

Assumption 2.1. Throughout this article we assume that there is a constant $\ell_0 > 0$ such that

$$\ell_e \geq \ell_0, \qquad e \in E, \tag{2.1}$$

i.e., that the weight function ℓ^{-1} is bounded. Without loss of generality, we also assume that $\ell_0 \leq 1$.

For each vertex $v \in V$ we set

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

i.e., $E_v^\pm$ consists of all edges starting $(-)$ resp. ending $(+)$ at v and E_v their *disjoint* union. Note that the *disjoint* union is necessary in order to allow self-loops, i.e., edges having the same initial and terminal point. The *degree of* $v \in V$ is defined as

$$\deg v := |E_v| = |E_v^+| + |E_v^-|,$$

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.

We want to introduce a vertex space allowing us to define Laplace-like combinatorial operators motivated by general vertex boundary conditions on quantum graphs. The usual discrete (weighted) Laplacian is defined on *scalar* functions $F\colon V \longrightarrow \mathbb{C}$ on the vertices V, namely

$$\Delta F(v) = -\frac{1}{\deg v} \sum_{e \in E_v} \frac{1}{\ell_e} \big(F(v_e) - F(v)\big), \tag{2.2}$$

where v_e denotes the vertex on e opposite to v. Note that Δ can be written as $\Delta = \mathsf{d}^*\mathsf{d}$ with

$$\mathsf{d}\colon \ell_2(V) \longrightarrow \ell_2(E), \qquad (\mathsf{d}F)_e = F(\partial_+ e) - F(\partial_- e), \tag{2.3}$$

where $\ell_2(V)$ and $\ell_2(E)$ carry the norms defined by

$$\|F\|^2_{\ell_2(V)} := \sum_{v \in V} |F(v)|^2 \deg v \quad \text{and} \quad \|\eta\|^2_{\ell_2(E)} := \sum_{e \in E} |\eta_e|^2 \frac{1}{\ell_e}, \tag{2.4}$$

and 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.

We would like to carry over the above concept for the vertex space $\ell_2(V)$ to more general vertex spaces $\mathscr{G}$. The main motivation to do so are metric graph Laplacians with general vertex boundary conditions as defined in Section 3 and their relations with discrete graphs (cf. Section 4).

Definition 2.2.

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

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

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

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

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

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

(iii) We call a general subspace $\mathscr{G}$ of $\mathscr{G}^{\max}$ *local* iff it decomposes with respect to the maximal vertex spaces, i.e., if $\mathscr{G} = \bigoplus_v \mathscr{G}_v$ and $\mathscr{G}_v \leq \mathscr{G}_v^{\max}$. Similarly, an operator A on $\mathscr{G}$ is called *local* if it is decomposable with respect to the above decomposition.

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

Note that a local subspace $\mathscr{G}$ is closed since $\mathscr{G}_v \leq \mathscr{G}_v^{\max}$ is finite dimensional. Alternatively, a vertex space is characterised by fixing an orthogonal projection P in $\mathscr{G}$ which is local.

Example 2.3. The names of the vertex spaces in the examples below will become clear in the quantum graph case. For more general cases, e.g. the discrete magnetic Laplacian, we refer to [P07b].

(i) Choosing $\mathscr{G}_v = \mathbb{C}\underline{\mathbb{1}}(v) = \mathbb{C}(1,\dots,1)$, we obtain the *continuous* or *standard* vertex space denoted by $\mathscr{G}_v^{\mathrm{std}}$. 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

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

(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.,

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

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

(iii) Assume that $\deg v = 4$ and define a vertex space of dimension 2 by

$$\mathscr{G}_v = \mathbb{C}(1,1,1,1) \oplus \mathbb{C}(1,\mathrm{i},-1,-\mathrm{i}).$$

The corresponding orthogonal projection is

$$P = \frac{1}{4}\begin{pmatrix} 2 & 1+\mathrm{i} & 0 & 1-\mathrm{i} \\ 1+\mathrm{i} & 0 & 1-\mathrm{i} & 2 \\ 0 & 1-\mathrm{i} & 2 & 1+\mathrm{i} \\ 1-\mathrm{i} & 2 & 1+\mathrm{i} & 0 \end{pmatrix}.$$

We will show some invariance properties of this vertex space in Example 2.14 (ii).

For the next definition, we need some more notation. Let $E_{0,v} \subset E_v$ be a subset of the set of adjacent edges at v. We denote by $\mathscr{G}_v\restriction_{E_{0,v}}$ the subspace of $\mathscr{G}_v$ where the coordinates *not* in $E_{0,v}$ are set to 0, i.e.,

$$\mathscr{G}_v\restriction_{E_{0,v}} := \{\, \underline{F}(v) \mid F_e(v) = 0, \quad \forall\, e \in E_v \setminus E_{0,v} \,\}.$$

Definition 2.4. A vertex space $\mathscr{G}_v$ at the vertex v is called *irreducible* if for any decomposition $E_v = E_{1,v} \cup E_{2,v}$ such that $\mathscr{G}_v = \mathscr{G}_v\restriction_{E_{1,v}} \oplus \mathscr{G}_v\restriction_{E_{2,v}}$ we have either $E_{1,v} = \emptyset$ or $E_{2,v} = \emptyset$. A vertex space $\mathscr{G}$ associated to a graph G is *irreducible* if all its components $\mathscr{G}_v$ are irreducible.

By definition, the minimal vertex space $\mathscr{G}_v^{\min} = 0$ is irreducible iff $\deg v = 1$.

In other words, a vertex space $\mathscr{G}_v$ is irreducible, if its projection P_v does not have block structure (in the given coordinates). The notion of *irreducibility* is useful in order to obtain a "minimal" representation of $\mathscr{G}$ by splitting a vertex with a reducible vertex space into several vertices. Repeating this procedure, we obtain:

Lemma 2.5. *For any vertex space $\mathscr{G}$ associated to a graph $G = (V, E, \partial)$, there exists a graph $\widetilde{G} = (\widetilde{V}, E, \widetilde{\partial})$ and a surjective graph morphism $\pi\colon \widetilde{G} \longrightarrow G$ such that $\mathscr{G}$ decomposes as*

$$\mathscr{G} = \bigoplus_{\widetilde{v}\in\widetilde{V}} \mathscr{G}_{\widetilde{v}} \quad \text{and} \quad \mathscr{G}_v = \bigoplus_{\widetilde{v}\in\pi^{-1}\{v\}} \mathscr{G}_{\widetilde{v}}.$$

In addition, each $\mathscr{G}_{\widetilde{v}}$ is irreducible.

Note that the edge set of $\widetilde{G}$ is the same as for the original graph G.

Proof. We construct the vertex set $\widetilde{V}$ of $\widetilde{G}$ as follows: Let $v \in V$ and $\mathscr{G}_v$ be an irreducible vertex space, then v is also an element of $\widetilde{V}$. Otherwise, if $\mathscr{G}_v = \mathscr{G}_v\restriction_{E_{1,v}} \oplus \mathscr{G}_v\restriction_{E_{2,v}}$ is a reducible vertex space

(for G), we replace the vertex v in V by two different vertices v_1, v_2 in $\widetilde{V}$ with adjacent edges $E_{1,v}$ and $E_{2,v}$, in particular, $\widetilde{G} = (V \setminus \{v\} \cup \{v_1, v_2\}, E, \widetilde{\partial})$ where

$$\widetilde{\partial}_\pm e = \begin{cases} \partial_\pm e, & \text{if } \partial_\pm e \neq v, \\ v_i, & \text{if } \partial_\pm = v \text{ and } e \in E_{v_i} \text{ for } i = 1, 2. \end{cases}$$

The associated vertex space at v_i is $\widetilde{\mathscr{G}}_{v_i} := \mathscr{G}_v\restriction_{E_{i,v}}$ for $i = 1, 2$. Repeating this procedure, we finally end with a graph $\widetilde{G}$ (denoted with the same symbol), such that each vertex space $\widetilde{\mathscr{G}}_{\widetilde{v}}$ is irreducible. The map π is defined by $\pi e = e$ and $\pi\widetilde{v} = v$ if $\widetilde{v}$ came from splitting a vertex space at the original vertex v. It is easy to see that π is a graph morphism (i.e, $\partial_\pm \pi e = \pi\widetilde{\partial}_\pm e$) and surjective. □

Definition 2.6. We call the graph $\widetilde{G}$ constructed in Lemma 2.5 the *irreducible* graph of the vertex space $\mathscr{G}$ associated to the graph G. We say that the vertex space is *connected* if the associated irreducible graph is a connected graph.

Note that on the level of the vertex space $\mathscr{G}$, passing to the irreducible graph is just a reordering of the coordinate labels, namely, a regrouping of the labels into smaller sets.

For example, the maximal vertex space $\mathscr{G}^{\max}$ associated to a graph G (with $\deg v \geq 2$ for all vertices v) is *not* irreducible, and its irreducible graph is

$$\widetilde{G} = \bigcup_{e\in E}^{\cdot} G_e \qquad \text{where} \qquad G_e := (\partial e, \{e\}, \partial\restriction_{\{e\}}) \tag{2.5}$$

is a graph with two vertices and one edge only. The vertex space is

$$\mathscr{G}^{\max} = \bigoplus_{e\in E} (\mathbb{C}_{\partial_- e} \oplus \mathbb{C}_{\partial_+ e}) \tag{2.6}$$

where $\mathbb{C}_{\partial_\pm e}$ is a copy of $\mathbb{C}$. The irreducible graph of the minimal vertex space $\mathscr{G}^{\min} = 0$ is the same as above.

However, the standard vertex space $\mathscr{G}^{\mathrm{std}}$ associated to a graph G is already irreducible and $\widetilde{G} = G$. Therefore, the standard vertex space is connected iff the underlying graph is connected; i.e., the notion of "connectedness" agrees with the usual one.

Now, we 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 2.7. Let $\mathscr{G}$ be a vertex space of the graph G. The *exterior derivative* on $\mathscr{G}$ is defined via

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

mapping 0-forms onto 1-forms.

We often drop the subscript $\mathscr{G}$ for the vertex space. The proof of the next lemma is straightforward (see e.g. [P07b, Lem. 3.3]):

Lemma 2.8. *Assume the lower lengths bound* (2.1)*, then* d *is norm-bounded by* $\sqrt{2/\ell_0}$*. The adjoint*

$$\mathsf{d}^* \colon \ell_2(E) \longrightarrow \mathscr{G}$$

fulfills the same norm bound and is given by

$$(\mathsf{d}^*\eta)(v) = P_v\Big(\Big\{\frac{1}{\ell_e}\,\widehat{\eta}_e(v)\Big\}\Big) \in \mathscr{G}_v,$$

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 2.9. The *discrete generalised Laplacian* associated to a vertex space $\mathscr{G}$ is defined as $\Delta_{\mathscr{G}} := \mathsf{d}^*_{\mathscr{G}}\mathsf{d}_{\mathscr{G}}$, i.e.,

$$(\Delta_{\mathscr{G}} F)(v) = P_v\Big(\Big\{\frac{1}{\ell_e}\big(F_e(v) - F_e(v_e)\big)\Big\}\Big)$$

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

Remark 2.10.

(i) From Lemma 2.8 it follows that $\Delta_{\mathscr{G}}$ is a bounded operator on $\mathscr{G}$ with norm estimated from above by $2/\ell_0$.
(ii) Note that the orientation of the edges plays no role for the "second order" operator $\Delta_{\mathscr{G}}$.
(iii) We can also define a Laplacian $\Delta^1_{\mathscr{G}} := \mathsf{d}_{\mathscr{G}}\mathsf{d}^*_{\mathscr{G}}$ acting on the space of "1-forms" $\ell_2(E)$ (and $\Delta^0_{\mathscr{G}} := \Delta_{\mathscr{G}} = \mathsf{d}^*_{\mathscr{G}}\mathsf{d}_{\mathscr{G}}$). For more details and the related supersymmetric setting, we refer to [P07b]. In particular, we have
$$\sigma(\Delta^1_{\mathscr{G}}) \setminus \{0\} = \sigma(\Delta^0_{\mathscr{G}}) \setminus \{0\}.$$
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]).
(iv) Assume that G is equilateral (i.e., $\ell_e = 1$), which implies $\sigma(\Delta_{\mathscr{G}}) \subseteq [0,2]$. Then using the 1-form Laplacian, one can show the spectral relation
$$\sigma(\Delta_{\mathscr{G}^\perp}) \setminus \{0,2\} = 2 - (\sigma(\Delta_{\mathscr{G}}) \setminus \{0,2\}),$$
i.e., if $\lambda \notin \{0,2\}$, then $\lambda \in \sigma(\Delta_{\mathscr{G}^\perp})$ iff $2-\lambda \in \sigma(\Delta_{\mathscr{G}})$ (cf. [P07b, Lem. 3.13 (iii)]).

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

Example 2.11.

(i) For the standard vertex space $\mathscr{G}^{\mathrm{std}}$, it is convenient to use the unitary transformation from $\mathscr{G}^{\mathrm{std}}$ onto $\ell_2(V)$ associating to $F \in \mathscr{G}$ the (common value) $\widetilde{F}(v) := F_e(v)$ as in Example 2.3 (i). Then the exterior derivative and its adjoint are unitarily equivalent to
$$\widetilde{\mathsf{d}}\colon \ell_2(V) \longrightarrow \ell_2(E), \qquad (\widetilde{\mathsf{d}}\widetilde{F})_e = \widetilde{F}(\partial_+ e) - \widetilde{F}(\partial_- e)$$
and
$$(\widetilde{\mathsf{d}}^*\eta)(v) = \frac{1}{\deg v} \sum_{e \in E_v} \frac{1}{\ell_e} \widehat{\eta}_e(v),$$
i.e., $\widetilde{\mathsf{d}}$ is the classical coboundary operator already defined in (2.3) and $\widetilde{\mathsf{d}}^*$ its adjoint.

Moreover, the corresponding discrete Laplacian $\Delta_{\mathscr{G}^{\mathrm{std}}}$ is unitarily equivalent to the usual discrete Laplacian $\Delta = \widetilde{\mathsf{d}}^*\widetilde{\mathsf{d}}$ defined in (2.2) as one can easily check.
(ii) Passing to the irreducible graph of a vertex space $\mathscr{G}$ is a reordering of the coordinate labels, and in particular, the Laplacian is the same (up to the order of the coordinate labels). Namely, for the minimal vertex space $\mathscr{G}^{\min} = 0$, we have $\mathsf{d} = 0$, $\mathsf{d}^* = 0$ and $\Delta_{\mathscr{G}^{\min}} = 0$.

For the maximal vertex space, we have
$$(\Delta_{\mathscr{G}^{\max}} F)_e(v) = \Big\{ \frac{1}{\ell_e} \big(F_e(v) - F_e(v_e) \big) \Big\}_{e \in E_v}$$
and
$$\Delta_{\mathscr{G}^{\max}} = \bigoplus_{e \in E} \Delta_{G_e} \qquad \text{where} \qquad \Delta_{G_e} \cong \frac{1}{\ell_e} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$
In particular, in both cases, the Laplacians are decoupled and any connection information of the graph is lost.

Of course, the decoupled minimal and maximal cases are uninteresting when analysing the graph and its properties. Moreover, it is natural to assume that the vertex space is connected and irreducible, since the other cases can be reduced to this one.

Let us analyse the generalised Laplacian in the special case when all lengths are equal, say, $\ell_e = 1$ and when there are no double edges. Then we can write the Laplacian in the form
$$\Delta_{\mathscr{G}} = \mathbb{1} - M_{\mathscr{G}}, \qquad M_{\mathscr{G}} := PA^{\max},$$

where $M_{\mathscr{G}}\colon \mathscr{G} \longrightarrow \mathscr{G}$ is called the *principle part* of the generalised discrete Laplacian, and $A^{\max}\colon \mathscr{G}^{\max} \longrightarrow \mathscr{G}^{\max}$ 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 $F \in \mathscr{G}^{\max}$. 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

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

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

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

Equivalently,

$$M_{\mathscr{G}} = \bigoplus_{v \in V} \sum_{w \in V} A_{\mathscr{G}}(v,w) \tag{2.7}$$

where the sum is actually only over those vertices w connected with v. In particular, in the standard case $\mathscr{G} = \mathscr{G}^{\mathrm{std}}$, the matrix $A_{\mathscr{G}^{\mathrm{std}}}(v,w)$ consists of one entry only since $\mathscr{G}_v^{\mathrm{std}} \cong \mathbb{C}(\deg v)$ isometrically, namely $A_{\mathscr{G}^{\mathrm{std}}}(v,w) = 1$ if v and w are connected and 0 otherwise, i.e., $A_{\mathscr{G}^{\mathrm{std}}}$ 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). In [P07b, Lem. 2.13] we showed the following result on symmetry of a vertex space:

Lemma 2.12. *Assume that the vertex space $\mathscr{G}_v$ of a vertex v with degree $d = \deg v$ is invariant under permutations of the coordinates $e \in E_v$, then $\mathscr{G}_v$ is one of the spaces $\mathscr{G}_v^{\min} = 0$, $\mathscr{G}^{\max} = \mathbb{C}^{E_v}$, $\mathscr{G}^{\mathrm{std}} = \mathbb{C}(1,\dots,1)$ or $(\mathscr{G}^{\mathrm{std}})^{\perp}$, i.e., only the minimal, maximal, standard and dual standard vertex space are invariant.*

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

Lemma 2.13. *Assume that the vertex space $\mathscr{G}_v$ of a vertex v with degree $d = \deg v$ is invariant under a cyclic permutation of the coordinates $e \in E_v = \{e_1,\dots,e_d\}$, i.e., edge $e_i \mapsto e_{i+1}$ and $e_d \mapsto e_1$, then $\mathscr{G}_v$ is an orthogonal sum of spaces of the form $\mathscr{G}_v^p = \mathbb{C}(1, \theta^p, \theta^{2p}, \dots, \theta^{(d-1)p})$ for $p = 0,\dots,d-1$, 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 $\mathscr{G}_v^p$ as given below. □

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

Example 2.14.

(i) If we require that the vertex space $\mathscr{G}_v$ is cyclic invariant with *real* coefficients in the corresponding projections, then $\mathscr{G}_v$ is $\mathbb{C}(1,\dots,1)$ or $\mathbb{C}(1,-1,\dots,1,-1)$ (if d even) or their sum. But the sum is reducible since

$$\mathscr{G}_v = \mathbb{C}(1,\dots,1) \oplus \mathbb{C}(1,-1,\dots,1,-1) = \mathbb{C}(1,0,1,0,\dots,1,0) \oplus \mathbb{C}(0,1,0,1,\dots,0,1)$$

and the latter two spaces are standard with degree $d/2$. In other words, the irreducible graph at v associated to the boundary space $\mathscr{G}_v$ 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 $\mathscr{G}_v = \mathscr{G}_v^0 \oplus \mathscr{G}_v^1 \leq \mathbb{C}^4$ of dimension 2 given in Example 2.3 (iii). Note that $\mathscr{G}_v$ is irreducible, since the associated projection P 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", i.e., $(1, \dots, 1)$ replaced by a sequence of non-zero numbers).

We finally develop an index theory associated to a vertex space $\mathscr{G}$. We define the Hilbert chain associated to a vertex space $\mathscr{G}$ as

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

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 as

$$H^0(G,\mathscr{G}) := \ker \mathsf{d}_{\mathscr{G}} \cong \ker \mathsf{d}_{\mathscr{G}} / \operatorname{ran} 0,$$
$$H^1(G,\mathscr{G}) := \ker \mathsf{d}_{\mathscr{G}}^* = \operatorname{ran} \mathsf{d}_{\mathscr{G}}^{\perp} \cong \ker 0 / \operatorname{ran} \mathsf{d}_{\mathscr{G}}$$

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 this cohomology is then defined as

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

i.e., the *Fredholm index* of $\mathsf{d}_{\mathscr{G}}$, provided at least one of the dimensions is finite. Note that for the standard vertex space $\mathscr{G}^{\mathrm{std}} \cong \ell_2(V)$, the exterior derivative is just (equivalent to) the classical coboundary operator defined in (2.3). In particular, the corresponding homology spaces are the classical ones, and $\dim H^p(G,\mathscr{G}^{\mathrm{std}})$ counts the number of components ($p = 0$) and edges not in a spanning tree ($p = 1$).

Using the stability of the index under (at least) continuous perturbations, we can calculate the index via simple (decoupled) model spaces and obtain (see [P07b, Sec. 4]):

Theorem 2.15. *Let $\mathscr{G}$ be a vertex space associated with the finite graph $G = (V, E, \partial)$, then*

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

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

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

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

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

since $\dim \mathscr{G}^{\max} = \sum_{v \in V} \deg v = 2|E|$ and $\dim \mathscr{G}^{\min} = 0$. Again, the index equals the Euler characteristic of the decoupled graph $\chi(\bigcup_e G_e)) = \sum_e \chi(G_e) = 2|E|$ (see Eq. (2.5)) resp. the relative Euler characteristic $\chi(G,V) = \chi(G) - \chi(V) = -|E|$.

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

Lemma 2.16. *Assume that the global length bound*

$$\ell_0 \leq \ell_e \leq \ell_+ \qquad \text{for all } \mathrm{e} \in E \tag{2.8}$$

holds for some constants $0 < \ell_0 \leq \ell_+ < \infty$. Then $H^0(G,\mathscr{G}^{\perp})$ and $H^1(G,\widehat{\mathscr{G}})$ are isomorphic. In particular, if G is finite, then $\operatorname{ind}(G,\mathscr{G}^{\perp}) = -\operatorname{ind}(G,\widehat{\mathscr{G}})$.

The change of orientation also occurs in the metric graph case, see e.g. Lemma 3.7.

3. Metric graphs

In this section, we fix the basic notion for metric and quantum graphs and derive some general assertion needed later on.

Definition 3.1. Let $G = (V, E, \partial)$ be a discrete graph. A *topological graph* associated to G is a CW complex X 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.

A *metric graph* $X = X(G, \ell)$ 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 $\Phi_e \colon \overline{I}_e \longrightarrow X$, $I_e := (0, \ell_e)$, whose image is the 1-cell corresponding to e, and the restriction $\Phi_e \colon I_e \longrightarrow \Phi(I_e) \subset X$ is a homeomorphism. The maps Φ_e induce a metric on X. In this way, X becomes a metric space.

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

$$X = \bigcup_{e \in E}^{\cdot} \overline{I}_e / \sim. \tag{3.1}$$

We denote the union of the 0-cells and the union of the (open) 1-cells (edges) by X^0 and X^1, i.e.,

$$X^0 = V \hookrightarrow X, \qquad X^1 = \bigcup_{e \in E} I_e \hookrightarrow X,$$

and both subspaces are canonically embedded in X.

Remark 3.2.

(i) The metric graph X becomes canonically a *metric measure space* by defining the distance of two points to be the length of the shortest path in X, joining these points. We can think of the maps $\Phi_e \colon I_e \longrightarrow X$ as coordinate maps and the Lebesgue measures on the intervals I_e induce a (Lebesgue) measure on the space X. We will often abuse the notion and write $X = (G, \ell)$ or $X = (V, E, \partial, \ell)$ for the metric graph associated to the weighted discrete graph (G, ℓ) with $G = (V, E, \partial)$.

(ii) Note that two metric graphs $X = (G, \ell)$, $X' = (G', \ell')$ can be isometric as metric spaces but not isomorphic as graphs: The metric on a metric graph X cannot distinguish between a single edge e of length ℓ_e in G and two edges e_1, e_2 of length ℓ_{e_1} , ℓ_{e_2} with $\ell_e = \ell_{e_1} + \ell_{e_2}$ joined by a single vertex of degree 2 in G': The underlying graphs are not (necessarily) isomorphic. For a discussion on this point, see for example [BaR07, Sec. 2].

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

$$\mathsf{L}_2(X) := \bigoplus_{e \in E} \mathsf{L}_2(I_e), \qquad f = \{f_e\}_e \quad \text{with } f_e \in \mathsf{L}_2(I_e) \text{ and}$$

$$\|f\|^2 = \|f\|^2_{\mathsf{L}_2(X)} := \sum_{e \in E} \int_{I_e} |f_e(x)|^2 \, \mathrm{d}x.$$

In order to define a natural Laplacian on $\mathsf{L}_2(X)$ we introduce the *maximal* or *decoupled* Sobolev space of order k as

$$\mathsf{H}^k_{\max}(X) := \bigoplus_{e \in E} \mathsf{H}^k(I_e),$$

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

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* value of f on the edge e at the vertex v by

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

Note that $\underline{f}_e(v)$ and $\widehat{\underline{f}}_e(v)$ are defined for $f \in \mathsf{H}^1_{\max}(X)$. Even more, we have shown in [P07b, Lem. 5.2] the following result:

Lemma 3.3. *Assume the lower lengths bound* (2.1)*, then the evaluation operators*

$$\underline{\bullet}\colon \mathsf{H}^1_{\max}(X) \longrightarrow \mathscr{G}^{\max} \quad \textit{and} \quad \widehat{\underline{\bullet}}\colon \mathsf{H}^1_{\max}(X) \longrightarrow \mathscr{G}^{\max},$$

given by $f \mapsto \underline{f} = \{\{\underline{f}_e(v)\}_{e\in E_v}\}_v \in \mathscr{G}^{\max} = \bigoplus_v \mathscr{G}^{\max}_v = \bigoplus_v \mathbb{C}^{E_v}$ *and similarly* $\widehat{\underline{f}} \in \mathscr{G}^{\max}$*, are bounded by* $2\ell_0^{-1/2}$*.*

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

$$\langle f', g\rangle_{\mathsf{L}_2(X)} = \langle f, -g'\rangle_{\mathsf{L}_2(X)} + \langle \underline{f}, \widehat{\underline{g}}\rangle_{\mathscr{G}^{\max}}, \tag{3.2}$$

where $f' = \{f'_e\}_e$ and similarly for g. Basically, this follows from partial integration on each interval I_e and a reordering of the labels by

$$E = \bigcup_{v\in V}^{\cdot} E_v^+ = \bigcup_{v\in V}^{\cdot} E_v^-.$$

Remark 3.4. 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 $\mathscr{G}$ be a vertex space (i.e., a local subspace of $\mathscr{G}^{\max}$, or more generally, a closed subspace) associated to the underlying discrete graph. We define

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

Note that these spaces are closed in $\mathsf{H}^k_{\max}(X)$ as pre-image of the bounded operators $\underline{\bullet}$ and $\widehat{\underline{\bullet}}$, respectively, of the closed subspace $\mathscr{G}$, and therefore itself Hilbert spaces.

We can now mimic the concept of exterior derivative:

Definition 3.5. The *exterior derivative* associated to a metric graph X and a vertex space $\mathscr{G}$ is the unbounded operator $\mathrm{d}_{\mathscr{G}}$ in $\mathsf{L}_2(X)$ defined by $\mathrm{d}_{\mathscr{G}} f := f'$ for $f \in \operatorname{dom} \mathrm{d}_{\mathscr{G}} := \mathsf{H}^1_{\mathscr{G}}(X)$.

Remark 3.6.

(i) Note that $\mathrm{d}_{\mathscr{G}}$ is a closed operator (i.e., its graph is closed in $\mathsf{L}_2(X) \oplus \mathsf{L}_2(X)$), since $\mathsf{H}^1_{\mathscr{G}}(X)$ is a Hilbert space and the graph norm of $\mathrm{d} = \mathrm{d}_{\mathscr{G}}$ given by $\|f\|^2_{\mathrm{d}} := \|\mathrm{d}f\|^2 + \|f\|^2$ is the Sobolev norm, i.e, $\|f\|_{\mathrm{d}} = \|f\|_{\mathsf{H}^1_{\max}(X)}$.

(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 boundary conditions $\underline{f} \in \mathscr{G}$, see also the next lemma.

The adjoint of $\mathrm{d}_{\mathscr{G}}$ can easily be calculated from the partial integration formula (3.2), namely the boundary term has to vanish for functions in the domain of $\mathrm{d}^*_{\mathscr{G}}$:

Lemma 3.7. *The adjoint of* $\mathrm{d}_{\mathscr{G}}$ *is given by* $\mathrm{d}^*_{\mathscr{G}} g = -g'$ *with domain* $\operatorname{dom} \mathrm{d}^*_{\mathscr{G}} = \mathsf{H}^1_{\widehat{\mathscr{G}}^\perp}(X)$.

As for the discrete operators, we define the Laplacian as

$$\Delta_{\mathscr{G}} := \mathrm{d}^*_{\mathscr{G}} \mathrm{d}_{\mathscr{G}}$$

with domain $\operatorname{dom} \Delta_{\mathscr{G}} := \{ f \in \operatorname{dom} \mathrm{d}_{\mathscr{G}} \,|\, \mathrm{d}f \in \operatorname{dom} \mathrm{d}^*_{\mathscr{G}} \}$. Moreover, we have (see e.g. [K04, Thm. 17] or [P07a, Sec. 5] for different proofs):

Proposition 3.8. *Assume the lower lengths bound* (2.1)*, then $\Delta_{\mathscr{G}}$ is self-adjoint on*

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

Proof. By definition of $\Delta_{\mathscr{G}}$, the Laplacian is the non-negative operator associated to the non-negative quadratic form $f \mapsto \|\mathrm{d}f\|^2$ with domain $\mathsf{H}^1_{\mathscr{G}}(X)$. The latter is closed since $\mathsf{H}^1_{\mathscr{G}}(X)$ is a Hilbert space equipped with the associated quadratic form norm defined by $\|f\|^2_{\mathsf{H}^1(X)} = \|\mathrm{d}f\|^2 + \|f\|^2$, see Remark 3.6 (i). It remains to show that $\Delta_{\mathscr{G}}$ is a closed operator, i.e., $\operatorname{dom}\Delta_{\mathscr{G}}$ is a Hilbert space equipped with the graph norm defined by $\|f\|^2_\Delta := \|f\|^2 + \|f''\|^2$. By Lemma 3.3, the domain is a closed subspace of $\mathsf{H}^2_{\max}(X)$, and it remains to show that the Sobolev and the graph norms

$$\|f\|^2_{\mathsf{H}^2_{\max}(X)} = \|f\|^2 + \|f'\|^2 + \|f''\|^2 \quad\text{and}\quad \|f\|^2_\Delta = \|f\|^2 + \|f''\|^2,$$

are equivalent, i.e., that there is a constant $C > 0$ such that $\|f'\|^2 \le C(\|f\|^2 + \|f''\|^2)$. The latter estimate is true under the global lower bound on the length function (2.1) (see e.g. [HP06, App. C]). □

Definition 3.9. A metric graph X together with a self-adjoint Laplacian (i.e, an operator acting as $(\Delta f)_e = -f_e''$ on each edge) will be called *quantum graph*.

For example, $(X, \Delta_{\mathscr{G}})$ is a quantum graph; defined by the data $(V, E, \partial, \ell, \mathscr{G})$.

Example 3.10. The standard vertex space $\mathscr{G}^{\mathrm{std}}$ leads to *continuous* functions in $\mathsf{H}^1_{\mathscr{G}^{\mathrm{std}}}(X)$, i.e., the value of $\underline{f}_e(v)$ is *independent* of $e \in E_v$. Note that on each edge, we already have the embedding $\mathsf{H}^1(I_e) \subset \mathsf{C}(I_e)$, i.e., f is already continuous inside each edge. In particular, a function f is in the domain of $\Delta_{\mathscr{G}^{\mathrm{std}}}$ iff $f \in \mathsf{H}^2_{\max}(X)$, f is continuous and $\widehat{\underline{f}'}(v) \in (\mathscr{G}^{\mathrm{std}})^\perp$. The latter condition on the derivative is a *flux* condition, namely

$$\sum_{e\in E_v} \widehat{\underline{f}'_e}(v) = 0$$

for all $v \in V$. The corresponding metric graph Laplacian $\Delta_{\mathscr{G}^{\mathrm{std}}}$ is called *standard*, or sometimes also *Kirchhoff* Laplacian.

Remark 3.11.

(i) There are other possibilities how to define self-adjoint extensions of a Laplacian, namely for any self-adjoint (bounded) operator L on $\mathscr{G}$, one can show that $\Delta_{(\mathscr{G},L)}$ is self-adjoint on

$$\operatorname{dom}\Delta_{(\mathscr{G},L)} := \big\{\, f \in \mathsf{H}^2_{\mathscr{G}}(X) \,\big|\, P\widehat{\underline{f}'} = L\underline{f} \,\big\},$$

where P is the projection in $\mathscr{G}^{\max}$ onto the space $\mathscr{G}$. The domain mentioned in Proposition 3.8 corresponds to the case $L = 0$. For more details, we refer e.g. to [K04, Thm. 17] or [P07a, Sec. 4], [KPS07] (and references therein) and the next remark for another way of a parametrisation of self-adjoint extensions.

(ii) One can encode the vertex boundary conditions also in a (unitary) operator S on $\mathscr{G}^{\max}$, the *scattering operator*. 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 $\Delta_{(\mathscr{G},L)}$ described above), one can show that S is independent of the *energy*, namely,

$$S = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} = 2P - \mathbb{1} \tag{3.3}$$

with respect to the decomposition $\mathscr{G}^{\max} = \mathscr{G} \oplus \mathscr{G}^\perp$, and where P is the orthogonal projection of $\mathscr{G}$ in $\mathscr{G}^{\max}$.

(iii) As in the discrete case, we can consider $\Delta^0_{\mathscr{G}} := \Delta_{\mathscr{G}}$ as the Laplacian on 0-forms, and $\Delta^1_{\mathscr{G}} := \mathrm{d}_{\mathscr{G}}\mathrm{d}^*_{\mathscr{G}}$ as the Laplacian on 1-forms, and again, by supersymmetry, we have the spectral relation

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

For more details and more general exterior derivatives corresponding to the case $L \geq 0$, we refer to [P07b, Sec. 5].

Using the definition $A \leq B$ iff $\operatorname{dom}\mathfrak{a} \supset \operatorname{dom}\mathfrak{b}$ and $\mathfrak{a}(f) \leq \mathfrak{b}(f)$ for all $f \in \operatorname{dom}\mathfrak{b}$ where $\mathfrak{a}$, $\mathfrak{b}$ are the quadratic forms associated to the self-adjoint (unbounded) non-negative operators A and B (i.e., $\mathfrak{a}(f) := \|A^{1/2}f\|^2 = \langle Af, f\rangle$ for $f \in \operatorname{dom}\mathfrak{a} := \operatorname{dom}A^{1/2}$ and $f \in \operatorname{dom}A$, respectively), we have the following simple observation:

Lemma 3.12. *Assume that $\mathscr{G}_1 \leq \mathscr{G}_2$ are two vertex spaces, then $\Delta_{\mathscr{G}_2} \leq \Delta_{\mathscr{G}_1}$.*

Proof. The assertion follows directly from the inclusion $\mathsf{H}^1_{\mathscr{G}_1}(X) \subset \mathsf{H}^1_{\mathscr{G}_2}(X)$ and the fact that the quadratic forms are given by $\mathfrak{d}_i(f) := \|\mathrm{d}f\|^2_{\mathsf{L}_2(X)}$ with $\operatorname{dom}\mathfrak{d}_i = \mathsf{H}^1_{\mathscr{G}_i}(X)$. □

If X is compact, i.e., the underlying graph is finite, we have:

Proposition 3.13. *Assume that X is compact, then the spectrum of $\Delta_{\mathscr{G}}$ is purely discrete, i.e., there is an infinite sequence $\{\lambda_k\}_k$ of eigenvalues where $\lambda_k = \lambda_k(\Delta_{\mathscr{G}}) = \lambda_k(\mathscr{G})$ denotes the k-th eigenvalue (repeated according to its multiplicity) and $\lambda_k \to \infty$ as $k \to \infty$.*

Proof. We have to show that the resolvent of $\Delta_{\mathscr{G}}$ is a compact operator. This assertion follows easily from the estimate $\Delta_{\mathscr{G}} \geq \Delta_{\mathscr{G}^{\max}} = \bigoplus_e \Delta^{\mathrm{N}}_{I_e}$ where $\Delta^{\mathrm{N}}_{I_e}$ is the Neumann Laplacian on the interval I_e having discrete spectrum $\lambda_k(\mathscr{G}^{\max}) = (k-1)^2\pi^2/\ell_e^2$ ($k = 1, 2, \dots$): The inequality implies the opposite inequality for the resolvents in -1; and therefore

$$0 \leq (\Delta_{\mathscr{G}} + 1)^{-1} \leq (\Delta_{\mathscr{G}^{\max}} + 1)^{-1} = \bigoplus_{e\in E} (\Delta^{\mathrm{N}}_{I_e} + 1)^{-1}.$$

Since E is finite, the latter operator is compact and therefore also the resolvent of $\Delta_{\mathscr{G}}$. □

Combining the last two results together with the variational characterisation of the eigenvalues (the min-max principle), we have the inequality

$$\lambda_k(\Delta_{\mathscr{G}_2}) \leq \lambda_k(\Delta_{\mathscr{G}_1})$$

for all $k \in \mathbb{N}$ where $\mathscr{G}_1 \leq \mathscr{G}_2$ are two vertex spaces. Moreover,

$$\lambda^{\mathrm{N}}_k\big(\dot{\bigcup_e} I_e\big) = \lambda_k(\Delta_{\mathscr{G}^{\max}}) \leq \lambda_k(\Delta_{\mathscr{G}}) \leq \lambda_k(\Delta_{\mathscr{G}^{\min}}) = \lambda^{\mathrm{D}}_k\big(\dot{\bigcup_e} I_e\big)$$

where $\lambda^{\mathrm{D}}_k\big(\dot{\bigcup}_e I_e\big)$ is the spectrum of the (decoupled) Dirichlet operator $\Delta_{\mathscr{G}^{\min}} = \bigoplus_e \Delta^{\mathrm{D}}_{I_e}$. Note that $\lambda^{\mathrm{N}}_k\big(\dot{\bigcup}_e I_e\big) = 0$ for $k = 1, \dots, |E|$, and $\lambda^{\mathrm{N}}_{k+|E|}\big(\dot{\bigcup}_e I_e\big) = \lambda^{\mathrm{D}}_k\big(\dot{\bigcup}_e I_e\big)$ where the latter sequence is a reordering of the individual Dirichlet eigenvalues $\lambda^{\mathrm{D}}_k(I_e) = k^2\pi^2/\ell_e^2$ repeated according to multiplicity. In particular, for an equilateral metric graph (i.e, $\ell_e = 1$ for all edges e), then

$$(m-1)^2\pi^2 \leq \lambda_k(\Delta_{\mathscr{G}}) \leq m^2\pi^2, \qquad k = (m-1)|E| + 1, \dots, m|E|,\ m = 1, 2, \dots$$

For non-compact metric graphs, we can characterise the spectrum via *generalised* eigenfunctions, i.e., functions $f\colon X \longrightarrow \mathbb{C}$ satisfying the local vertex conditions $\underline{f}(v) \in \mathscr{G}_v$ and $\widehat{\underline{f}}(v) \in \mathscr{G}_v^\perp$, but no integrability condition at infinity: A measure ρ on $\mathbb{R}$ is a *spectral measure* for $\Delta_{\mathscr{G}}$ iff for all measurable $I \subset \mathbb{R}$ we have $\rho(I) = 0$ iff the spectral projector satisfies $\mathbb{1}_I(\Delta_{\mathscr{G}}) = 0$. In this case, we have the following result (cf. [HP06, App. B]):

Proposition 3.14. *Assume the lower lengths bound (2.1). Let $\Phi\colon X \longrightarrow (0, \infty)$ be a bounded weight function, which is also in $\mathsf{L}_2(X)$. Then for almost every $\lambda \in \sigma(\Delta_{\mathscr{G}})$ (with respect to a spectral measure), there is a generalised eigenfunction $f = f_\lambda$ associated to λ such that*

$$\|\Phi f\|^2 = \int_X |f(x)|^2\Phi(x)^2\,\mathrm{d}x < \infty.$$

The function Φ can be constructed according to the graph. Denote by $B_X(x_0, r)$ the metric ball of radius $r > 0$ around the point $x_0 \in X$. For example, on a graph with sub-exponential volume growth, i.e., for any $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$\operatorname{vol}_1 B_X(x_0, r) := \int_X \mathbb{1}_{B_X(x_0,r)} \,\mathrm{d}x \leq C_\varepsilon \mathrm{e}^{\varepsilon r},$$

the weight function Φ can be chosen in such a way that it decays slower than exponentially, i.e., $\min \Phi(B_X(x_0, r)) \geq \widetilde{C}_\varepsilon \mathrm{e}^{-\varepsilon r}$. In particular, we can choose $\Phi(x) := \mathrm{e}^{-\varepsilon d(x,x_0)} \leq 1$, and, by Fubini, $\|\Phi\|^2$ equals

$$\int_0^1 \operatorname{vol}_1\{\, x \in X \mid \Phi(x)^2 > t \,\} \,\mathrm{d}t = \int_0^1 \operatorname{vol}_1 B_X\Big(x_0, \frac{-\log t}{2\varepsilon}\Big) \,\mathrm{d}t \leq C_\varepsilon \int_0^1 t^{-1/2} \,\mathrm{d}t < \infty.$$

4. Relations between discrete and metric graphs

In this section, we describe two cases, in which (parts of the) spectrum of a metric graph can be described in terms of the discrete graph. The first case deals with so-called *equilateral* metric graphs, i.e., graphs where all lengths are the same, say, $\ell_e = 1$. The second case treats the spectrum at the bottom, also in the *general* (non-equilateral) case.

4.1. **Equilateral metric graphs.** An effective way of describing the relation between metric graph Laplacians and the underlying (generalised) discrete one are so-called *boundary triples*. We do not give the general definition here. instead, we refer to [P07a, BGP08] and the references therein. In brief, a boundary triple (originally developped for PDE boundary value problems) describes an abstraction of Green's formula.

In order to describe the notions needed here, we define a *maximal* Laplacian in $\mathscr{H} := \mathsf{L}_2(X)$ with domain

$$\operatorname{dom} \Delta_{\mathscr{G}}^{\max} := \mathsf{H}^2_{\mathscr{G}}(X) = \big\{\, f \in \mathsf{H}^2_{\max}(X) \,\big|\, \underline{f} \in \mathscr{G} \,\big\},$$

i.e., we only fix the vertex values $\underline{f}$ to be in the vertex space $\mathscr{G}$ with associated projection P. One can show similarly as in the proof of Proposition 3.8 that $\operatorname{dom} \Delta_{\mathscr{G}}^{\max}$ is a closed operator.

We define the boundary operators on the domain of the maximal Laplacian as

$$\Gamma_0 \colon \mathsf{H}^2_{\mathscr{G}}(X) \longrightarrow \mathscr{G}, \qquad f \mapsto \underline{f} \tag{4.1a}$$

$$\Gamma_1 \colon \mathsf{H}^2_{\mathscr{G}}(X) \longrightarrow \mathscr{G}, \qquad f \mapsto P\widehat{\underline{f}'}. \tag{4.1b}$$

Green's formula in this setting reads as

$$\langle \Delta_{\mathscr{G}}^{\max} f, g\rangle_{\mathscr{H}} - \langle f, \Delta_{\mathscr{G}}^{\max} g\rangle_{\mathscr{H}} = \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathscr{G}} - \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathscr{G}}$$

as one can easily see with the help of (3.2). As self-adjoint reference operator, we denote by Δ_0 the restriction of $\Delta_{\mathscr{G}}^{\max}$ to $\ker \Gamma_0$. Note that Δ_0 is precisely the metric graph Laplacian associated to the minimal vertex space $\mathscr{G}^{\min} = 0$, and therefore decoupled, i.e.,

$$\Delta_0 = \bigoplus_{e \in E} \Delta_{I_e}^{\mathrm{D}},$$

where $\Delta_{I_e}^{\mathrm{D}}$ denotes the Laplacian on I_e with Dirichlet boundary conditions and spectrum given by $\sigma(\Delta_{I_e}^{\mathrm{D}}) = \{\, (\pi k/\ell_e)^2 \mid k = 1, 2, \dots \,\}$ and $\sigma(\Delta_0)$ is the union of all these spectra.

In the general theory of boundary triples, one can show that Γ_0 restricted to $\mathscr{N}^z = \ker(\Delta_{\mathscr{G}}^{\max} - z))$ is a topological isomorphism between $\mathscr{N}^z$ and $\mathscr{G}$ provided $z \notin \sigma(\Delta_0) =: \Sigma$. We denote its inverse by $\beta(z) \colon \mathscr{G} \longrightarrow \mathscr{N}^z \subset \mathsf{L}_2(X)$ (*Krein's* Γ*-field*). In other words, $f = \beta(z)F$ is the solution of the Dirichlet problem

$$(\Delta - z)f = 0, \qquad \underline{f} = F.$$

Here, we can give an explicit formula for $\beta(z)$, namely we have

$$f_e(x) = F_e(\partial_- e) s_{-,e,z}(x) + F_e(\partial_+ e) s_{+,e,z}(x),$$

where[1]

$$s_{-,e,z}(x) = \frac{\sin(\sqrt{z}(\ell_e - x))}{\sin\sqrt{z}\ell_e} \quad \text{and} \quad s_{+,e,z}(x) = \frac{\sin(\sqrt{z}x)}{\sin\sqrt{z}\ell_e}. \tag{4.2}$$

denote the fundamental solutions for $z \notin \sigma(\Delta_0)$.

Taking the derivative of $f = \beta(z)F$ on $\mathscr{G}$, i.e., defining

$$Q(z)F := \Gamma_1\beta(z)F,$$

we obtain a (bounded) operator $Q(z)\colon \mathscr{G} \longrightarrow \mathscr{G}$, called *Krein's Q-function* or *Dirichlet-to-Neumann map*. Here, a simple calculation shows that

$$(Q(z)F)_e(v) = \frac{\sqrt{z}}{\sin(\sqrt{z}\ell_e)}\big[\cos(\sqrt{z}\ell_e)F_e(v) - F_e(v_e)\big].$$

if $z \notin \Sigma$. In particular, if the metric graph is equilateral (without loss of generality, $\ell_e = 1$), we have

$$Q(z) = \frac{\sqrt{z}}{\sin\sqrt{z}}\big[\boldsymbol{\Delta}_{\mathscr{G}} - (1 - \cos\sqrt{z})\big].$$

The abstract theory of boundary triples gives here the following result between the metric and discrete Laplacian. For a proof and more general self-adjoint Laplacians as in Remark 3.11 (i) we refer to [P07a, Sec. 5]. Certain special cases can be found for example in [C97, Pa06, BGP08]; and Pankrashkin announced a more general result in [Pa07]. For a related result concerning a slightly different definition of a metric graph Laplacian, see [BaF06] and the references therein. For spectral relations concerning averaging operators we refer to [CaW05].

Theorem 4.1. *Assume the lower bound on the edge lengths* (2.1).

(i) *For $z \notin \sigma(\Delta_0)$ we have the explicit formula for the eigenspaces*

$$\ker(\Delta_{\mathscr{G}} - z) = \beta(z)\ker Q(z).$$

(ii) *For $z \notin \sigma(\Delta_{\mathscr{G}}) \cup \sigma(\Delta_0)$ we have $0 \notin \sigma(Q(z))$ and Krein's resolvent formula*

$$(\Delta_{\mathscr{G}} - z)^{-1} = (\Delta_0 - z)^{-1} - \beta(z)Q(z)^{-1}(\beta(\overline{z}))^*$$

holds.

(iii) *Assume that the graph is equilateral (say, $\ell_e = 1$), then for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ or $\lambda \in \mathbb{R}$ in the spectral gap $(\pi^2k^2, \pi^2(k+1)^2)$ $(k = 1, 2, \dots)$ of Δ_0 or $\lambda < \pi^2$, we have*

$$(\Delta_{\mathscr{G}} - \lambda)^{-1} = (\Delta_0 - \lambda)^{-1} - \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}}\beta(\lambda)\big(\boldsymbol{\Delta}_{\mathscr{G}} - (1 - \cos\sqrt{\lambda})\big)^{-1}(\beta(\overline{\lambda}))^*$$

and

$$\lambda \in \sigma_\bullet(\Delta_{\mathscr{G}}) \;\Leftrightarrow\; (1 - \cos\sqrt{\lambda}) \in \sigma_\bullet(\boldsymbol{\Delta}_{\mathscr{G}})$$

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

Remark 4.2. (i) The eigenspaces in Theorem 4.1 (i) for an equilateral graph can be constructed from the discrete data $F \in \ker(\boldsymbol{\Delta}_{\mathscr{G}} - (1 - \cos\sqrt{z}))$ by applying Krein's Γ-function, the "solution operator", namely, $f = \beta(z)F$ is the corresponding eigenfunction of the metric graph Laplacian. The converse is also true: Given $f \in \ker(\Delta_{(\mathscr{G},0)} - z)$, then the corresponding eigenfunction $F \in \ker(\boldsymbol{\Delta}_{\mathscr{G}} - (1 - \cos\sqrt{z}))$ is just the restriction of f to the vertices, namely $F = \underline{f}$.

[1]For $z = 0$, we set $s_{-,e,0}(x) := 1 - x/\ell_e$ and $s_{+,e,0}(x) := x/\ell_e$.

(ii) The resolvent formula in Theorem 4.1 (ii) is very explicit, since

$$(\Delta_0 - z)^{-1} = \bigoplus_{e\in E} (\Delta_{I_e}^{\mathrm{D}} - z)^{-1}$$

is decoupled and explicit formulas for the resolvent on the interval are known. In particular, the analysis of the (equilateral) metric graph resolvent is reduced to the analysis of the discrete Laplacian resolvent (see also [KoS06, KPS07]).

Krein's resolvent formula (ii) is very useful when analysing further properties of the quantum graph $(X, \Delta_{\mathscr{G}})$ via the resolvent.

(iii) We excluded the Dirichlet spectrum $\sigma(\Delta_0) = \Sigma$. These values may occur in the spectrum of $\Delta_{\mathscr{G}}$ or not. For example, if $\mathscr{G}$ is the standard vertex space $\mathscr{G}^{\mathrm{std}}$ and if X contains a loop with an even number of edges each having the same length, we can define on each edge a Dirichlet solution on the edge (with opposite sign on successive edges). This function is continuous in the vertices, and satisfies also the Kirchhoff condition in each vertex. Therefore, on a metric graph, compactly supported eigenfunctions may exist.

4.2. **Relation at the bottom of the spectrum.** Let us analyse the spectrum at the bottom in more detail. As in Section 2 we define the Hilbert chain associated to the exterior derivative $\mathrm{d}_{\mathscr{G}}$ as

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

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

$$H^0(X,\mathscr{G}) := \ker \mathrm{d}_{\mathscr{G}} \cong \ker \mathrm{d}_{\mathscr{G}} / \operatorname{ran} 0,$$
$$H^1(X,\mathscr{G}) := \ker \mathrm{d}^*_{\mathscr{G}} = \operatorname{ran} \mathrm{d}^{\perp}_{\mathscr{G}} \cong \ker 0 / \operatorname{ran} \mathrm{d}_{\mathscr{G}}$$

The *index* or *Euler characteristic* of the cohomology associated to the metric graph X with vertex space $\mathscr{G}$ is then defined as

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

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

We have the following result (for more general cases cf. [P07b], and for a different approach see [FKW07]):

Theorem 4.3. *Assume that G is a weighted discrete graph with lower lengths bound* (2.1)*, and denote by X the associated metric graph, and by $\mathscr{G}$ a vertex space associated to G. Then there is an isomorphism $\Phi^* = \Phi_0^* \oplus \Phi_1^*$ with*

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

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

$$\begin{array}{ccccccccc}
\mathscr{C}_{X,\mathscr{G}}\colon 0 & \longrightarrow & \mathsf{H}^1_{\mathscr{G}}(X) & \xrightarrow{\mathrm{d}_{\mathscr{G}}} & \mathsf{L}_2(X) & \longrightarrow & 0 \\
 & & \downarrow{\scriptstyle \Phi_0} & & \downarrow{\scriptstyle \Phi_1} & & \\
\mathscr{C}_{G,\mathscr{G}}\colon 0 & \longrightarrow & \mathscr{G} & \xrightarrow{\mathsf{d}_{\mathscr{G}}} & \ell_2(E) & \longrightarrow & 0
\end{array}$$

is commutative, where

$$\Phi_0 f := \underline{f} = \Gamma_0 f, \qquad \Phi_1 g := \left\{ \int_{I_e} g_e(x)\,\mathrm{d}x \right\}_e.$$

In particular, if G is finite (and therefore X compact), then

$$\operatorname{ind}(G,\mathscr{G}) = \operatorname{ind}(X,\mathscr{G}).$$

For general results on Hilbert chains and their morphisms we refer to [L02, Ch. 1] or [BL92].

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

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

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

$$\begin{array}{ccccccccc}
\mathscr{C}_{X,\mathscr{G}}\colon & 0 & \longrightarrow & \mathsf{H}^1_{\mathscr{G}}(X) & \xrightarrow{\mathrm{d}_{\mathscr{G}}} & \mathsf{L}_2(X) & \longrightarrow & 0 \\
 & & & \uparrow{\scriptstyle \Psi_0} & & \uparrow{\scriptstyle \Psi_1} & & \\
\mathscr{C}_{G,\mathscr{G}}\colon & 0 & \longrightarrow & \mathscr{G} & \xrightarrow{\mathsf{d}_{\mathscr{G}}} & \ell_2(E) & \longrightarrow & 0
\end{array}$$

given by

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

(see Eq. (4.2)), i.e., we let $\Phi_0 F$ be the affine (harmonic) function on I_e with boundary values fixed; and $\Phi_1\eta$ be an (edgewise) constant function. Again, the chain morphism property $\Psi_1 \mathsf{d}_{\mathscr{G}} = \mathrm{d}_{\mathscr{G}} \Psi_0$ can easily be seen. Furthermore, $\Phi\Psi$ is the identity on the second (discrete) Hilbert chain $\mathscr{C}_{G,\mathscr{G}}$. 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 4.4. The sub-complex $\Psi(\mathscr{C}_{G,\mathscr{G}})$ of $\mathscr{C}_{X,\mathscr{G}}$ consists of the subspace of edge-wise affine 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 $0 < \ell_0 \le \ell_e \le \ell_+ < \infty$, then

$$\begin{aligned}
\|\Psi_0 F\|^2 = \sum_e \frac{1}{\ell_e} \int_0^{\ell_e} |F_e(\partial_- e)(\ell_e - x) + F_e(\partial_+ e)x|^2\,\mathrm{d}x \\
= \sum_e \frac{1}{3\ell_e} \int_0^{\ell_e} |F_e(\partial_- e)^2 + F_e(\partial_- e)F_e(\partial_+ e) + F_e(\partial_+ e)^2|,
\end{aligned}$$

so that

$$\frac{1}{2\ell_+}\|F\|_{\mathscr{G}}^2 \le \|\Psi_0 F\|^2 \le \frac{5}{6\ell_0}\|F\|_{\mathscr{G}}^2,$$

i.e., redefining the norm on $\mathscr{G}$ by $\|F\|_{\mathscr{G},1} := \|\Psi_0 F\|$ 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.

5. Relations between metric graphs and manifolds

Let us briefly describe the relation of a metric graph $X_0 = (V, E, \partial, \ell)$ with manifolds. For more details, we refer to the review article [EP07] and the references therein. Let X_ε be a d-dimensional connected manifold with metric g_ε. If X_ε has boundary, we denote it by ∂X_ε; let us stress that our discussion covers different kind of models, like the ε-neighbourhood of an metric graph *embedded* in $\mathbb{R}^\nu$, as well as sleeve-type manifolds (like the surface of a pipeline network) having no boundary. We assume that X_ε can be decomposed into open sets $U_{\varepsilon,e}$ and $U_{\varepsilon,v}$, i.e.,[2]

$$X_\varepsilon = \dot{\bigcup_{e\in E}} U_{\varepsilon,e} \;\dot\cup\; \dot{\bigcup_{v\in V}} U_{\varepsilon,v}. \tag{5.1}$$

[2] The expression $A = \dot\bigcup_i A_i$ means that the A_i's are open (in A), mutually disjoint and the interior of $\bigcup_i \overline{A}_i$ equals A.

Denote the metric on X_ε by g_ε. To simplify the discussion here, we assume that $U_{\varepsilon,e}$ and $U_{\varepsilon,v}$ are isometric to

$$U_{\varepsilon,e} \cong (I_e \times F, g_{\varepsilon,e}) \qquad g_{\varepsilon,e} = \mathrm{d}x_e^2 + \varepsilon^2 h \tag{5.2a}$$

$$U_{\varepsilon,v} \cong (U_v, g_{\varepsilon,v}) \qquad g_{\varepsilon,v} = \varepsilon^2 g_v \tag{5.2b}$$

where (F, h) is a compact m-dimensional manifold with $m := (d-1)$, and (U_v, g_v) is an ε-independent d-dimensional manifold (cf. Figure 1). Strictly speaking, for a metric graph X_0 embedded in $\mathbb{R}^2$, the edge neighbourhoods of the associated ε-neighbourhood $X_\varepsilon := \{\, x \in \mathbb{R}^2 \,|\, \operatorname{dist}(x, X_0) < \varepsilon \,\}$ must be shorter in the longitudinal direction in order to have space for the vertex neighbourhoods. Nevertheless, this fact causes only an error of order ε for the associated metrics, which does not matter in our convergence analysis below.

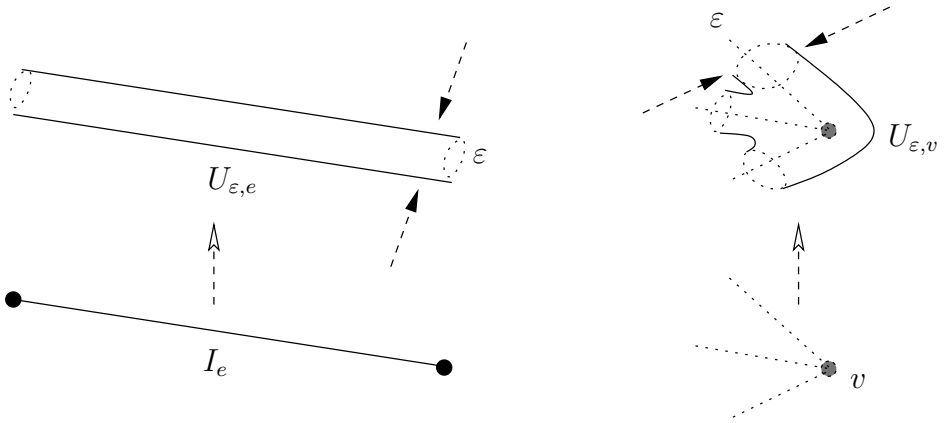

FIGURE 1. The associated edge and vertex neighbourhoods with $F_\varepsilon = \mathbb{S}^1_\varepsilon$, i.e., $U_{\varepsilon,e}$ and $U_{\varepsilon,v}$ are 2-dimensional manifolds with boundary.

Note that $\partial U_{\varepsilon,v} \setminus \partial X_\varepsilon$ has $(\deg v)$-many components isometric to $(F, \varepsilon^2 h)$ denoted by $(\partial_e U_v, \varepsilon^2 h)$ for $e \in E_v$. The cross section manifold F has a boundary or does not have one, depending on the analogous property of X_ε.

On the other hand, given a metric graph X_0 and vertex neighbourhood manifolds U_v as below, we can abstractly construct a graph-like manifold X_1 from these building blocks according to the rules of the graph with a family of metrics g_ε satisfying (5.1) and (5.2) with $X_\varepsilon = (X_1, g_\varepsilon)$.

For simplicity, we suppose that $\operatorname{vol}_m F = 1$. Then we have

$$\mathrm{d}U_{\varepsilon,e} = \varepsilon^m \,\mathrm{d}F \,\mathrm{d}x_e \tag{5.3}$$

for the Riemannian densities. We consider the Hilbert space $\mathscr{H}_\varepsilon = \mathsf{L}_2(X_\varepsilon)$ and the Laplacian $\Delta_{X_\varepsilon} := \mathrm{d}^*\mathrm{d} \geq 0$ (with Neumann boundary conditions if $\partial X_\varepsilon \neq \emptyset$) where d denotes the exterior derivative. In addition, we assume that the following uniformity conditions are valid,

$$c_{\mathrm{vol}} := \sup_{v \in V} \operatorname{vol}_d U_v < \infty, \qquad \lambda_2 := \inf_{v \in V} \lambda_2^{\mathrm{N}}(U_v) > 0, \tag{5.4}$$

where $\lambda_2^{\mathrm{N}}(U_v)$ denotes the second (i.e., first non-zero) Neumann eigenvalue of (U_v, g_v). Roughly speaking, the requirements (5.4) mean that the region U_v remains small w.r.t. the vertex index. Obviously, these assumptions are trivially satisfied once the vertex set V is finite.

In order to compare operators in $\mathsf{L}_2(X_0)$ and $\mathsf{L}_2(X_\varepsilon) = \bigoplus_e \mathsf{L}_2(I_e) \otimes \mathsf{L}_2(F_\varepsilon) \oplus \bigoplus_v \mathsf{L}_2(U_{\varepsilon,v})$, we use the identification operator

$$Jf := \{f_e \otimes \mathbb{1}_\varepsilon\}_e \oplus \{0_v\}_v, \tag{5.5}$$

where $\mathbb{1}_\varepsilon = \varepsilon^{-m/2}\mathbb{1}$ is the lowest normalised eigenfunction on $F_\varepsilon = (F, \varepsilon^2 h)$ and in turn 0_v is the zero function on U_v. This identification operator is *quasi-unitary*, i.e., $J^*J = \mathrm{id}_{\mathscr{H}_0}$, $\|J\| = 1$, and one can show that

$$\|(JJ^* - \mathrm{id}_{\mathscr{H}_\varepsilon})(\Delta_{X_\varepsilon} + 1)^{-1/2})\| = \mathscr{O}(\varepsilon^{1/2}),$$

where $\mathscr{O}(\varepsilon^{1/2})$ depends only on the lower lengths bound ℓ_0 in (2.1), on c_{vol} and λ_2: Basically, we have

$$(\mathrm{id}_{\mathscr{H}_\varepsilon} - JJ^*)u = \sum_{e\in E} \int_{I_e} \|u(x,\cdot) - \langle u(x,\cdot), \mathbb{1}_\varepsilon\rangle_{F_{\mathrm{e}\varepsilon}}\|^2_{F_\varepsilon}\,\mathrm{d}x + \sum_{v\in V} \|u\|^2_{U_{\varepsilon,v}}$$

and both contributions can be estimated in terms of $\mathscr{O}(\varepsilon)(\|\mathrm{d}u\|^2 + \|u\|^2)$ as stated above.

The main statement of this section is the following (cf. [P06]):

Theorem 5.1. *Assume the uniformity conditions* (2.1), $d_0 := \sup_v \deg v < \infty$ *and* (5.4). *Then the Laplacians* Δ_{X_ε} *and* Δ_{X_0} *are* $\mathscr{O}(\varepsilon^{1/2})$*-close with respect to the quasi-unitary map* J *defined in* (5.5)*, i.e.*

$$\|(\Delta_{X_\varepsilon} + 1)^{-1}J - J(\Delta_{X_0} + 1)^{-1}\| \le \mathscr{O}(\varepsilon^{1/2}).$$

In addition, we have

$$\|(\Delta_{X_\varepsilon} + 1)^{-1} - J(\Delta_{X_0} + 1)^{-1}J^*\| \le \mathscr{O}(\varepsilon^{1/2}), \tag{5.6}$$

where the error term depends only on ℓ_0*,* d_0*,* c_{vol} *and* λ_2*.*

Once the above resolvent estimates are established, one can develop a functional calculus for pairs of operators $(\mathscr{H}_\varepsilon, \Delta_{X_\varepsilon})$ and $(\mathscr{H}_0, \Delta_{X_0})$ together with a quasi-unitary identification operator J, and establish the above operator estimates also for more general functions φ than $\varphi(\lambda) = (\lambda+1)^{-1}$, namely for spectral projectors ($\varphi = \mathbb{1}_I$, I interval), or for the heat operator ($\varphi_t(\lambda) = \mathrm{e}^{-t\lambda}$, $t > 0$). Moreover, we can show that the spectra are close to each other:

Theorem 5.2. *Under the assumptions of the previous theorem, we have*

$$\|\mathbb{1}_I(\Delta_{X_\varepsilon})J - J\mathbb{1}_I(\Delta_{X_0})\| \le \mathscr{O}(\varepsilon^{1/2}) \quad \textit{and} \quad \|\mathbb{1}_I(\Delta_{X_\varepsilon}) - J\mathbb{1}_I(\Delta_{X_0})J^*\| \le \mathscr{O}(\varepsilon^{1/2})$$

for the spectral projections provided I *is a compact interval such that* $\partial I \cap \sigma(\Delta_{X_0}) = \emptyset$*. In particular, if* I *contains a single eigenvalue* $\lambda(0)$ *of* Δ_{X_0} *with multiplicity one corresponding to an eigenfunction* $u(0)$*, then there is an eigenvalue* $\lambda(\varepsilon)$ *and an eigenfunction* $u(\varepsilon)$ *of* Δ_{X_ε} *such that*

$$\|Ju(0) - u(\varepsilon)\| = \mathscr{O}(\varepsilon^{1/2}).$$

In addition, the spectra converge uniformly on $[0,\Lambda]$*, i.e.*

$$\sigma(\Delta_{X_\varepsilon}) \cap [0,\Lambda] \to \sigma(\Delta_{X_0}) \cap [0,\Lambda]$$

in the sense of the Hausdorff distance on compact subsets of $[0,\Lambda]$*. The same result is true if we consider only the essential or the discrete spectral components.*

In particular, the above theorem applies to the case when X_0 (and therefore X_ε) is compact, and we obtain

$$\lambda_k(\Delta_{X_\varepsilon}) - \lambda_k(\Delta_{X_0}) = \mathscr{O}(\varepsilon^{1/2}). \tag{5.7}$$

This estimate can also be proved directly by applying the min-max theorem, and estimating the errors of the corresponding Rayleigh quotients. For more results (like a similar convergence of resonances) we refer again to [EP07] and the references therein. Recently, Grieser showed in [Gr07] an asymptotic expansion of the eigenvalues and the eigenfunctions also for other boundary conditions on ∂X_ε, for example Dirichlet.

6. Estimates on the first non-zero eigenvalue

Here, we comment on inequalities on the first non-zero eigenvalue of a graph, namely a lower bound in terms of an isoperimetric constant. For details, see e.g. [Ch97, HSh04, N87].

Let X be a compact metric graph and $Y \subset X$ be a non-empty open subset. We denote by $|\partial Y|$ the number of points in the boundary ("volume" of dimension 0), and by $\mathrm{vol}_1 Y := \int_X \mathbb{1}_Y\,\mathrm{d}x$ the total length of Y ("volume" of dimension 1). *Cheeger's (isoperimetric) constant* for the metric graph X is defined as

$$h(X) := \inf_Y \frac{|\partial Y|}{\min(\mathrm{vol}_1 Y, \mathrm{vol}_1 Y^{\mathrm{c}})} \tag{6.1}$$

where $Y^{\mathrm{c}} := X \setminus Y$, and the infimum runs over all open, subset $Y \subset X$ such that $Y \neq \emptyset$ and $Y \neq X$.

For simplicity, we assume that X is connected and that each vertex space is standard, i.e., $\mathscr{G}_v = \mathscr{G}^{\mathrm{std}} = \mathbb{C}(1, \dots, 1)$. The corresponding (standard or Kirchhoff) Laplacian (denoted by Δ_X^{std}) has discrete spectrum. In particular, the first eigenvalue fulfills $\lambda_1(\Delta_X^{\mathrm{std}}) = 0$, while the second is positive $\lambda_2(X) := \lambda_2(\Delta_X^{\mathrm{std}}) > 0$. If not already obvious, this follows from Theorem 4.3, and the fact that the dimension of the 0-th cohomology group counts the number of components.

Cheeger's theorem in this context is the following:

Theorem 6.1. *Assume that X is a connected, compact metric graph with standard vertex space $\mathscr{G}^{\mathrm{std}}$ and denote by $\lambda_2(X) > 0$ the first non-zero eigenvalue of the standard (Kirchhoff) metric graph Laplacian. Then we have*

$$\lambda_2(X) \geq \frac{h(X)^2}{4}.$$

Proof. The proof follows closely the line of arguments as in the manifold case (see also [N87]). The basic ingredient is the *co-area formula*

$$\int_X |\varphi'(x)| \, \mathrm{d}x = \int_0^\infty |\{ x \in X \mid \varphi(x) = t \}| \, \mathrm{d}t$$

for any non-negative, edgewise C^1-function φ.

Denote by f the corresponding eigenfunction associated to $\lambda_2(X)$. Without loss of generality, we may assume that f is real-valued. Set $X_+ := \{ x \in X \mid f(x) > 0 \}$. Moreover, we may assume that $\mathrm{vol}_1 X_+ \leq \mathrm{vol}_1 X_+^{\mathrm{c}}$ (if this is not true, replace f by $-f$). Finally, $X_+ \neq \emptyset$ and $X_+ \neq X$ since f changes sign as second eigenfunction (only the first eigenfunction is constant).

Let $g := \mathbb{1}_{X_+} f$, then g is non-negative and $g \neq 0$. Moreover, since g is continuous, we can perform partial integration without additional boundary terms in ∂X_+: In particular, if $v \in \partial X_+$ is a vertex then $g_e(v) = 0$ for all adjacent edges $e \in E_v$. In particular, we have

$$\lambda_2(X) = \frac{\langle g, -g'' \rangle}{\|g\|^2} = \frac{\|g'\|^2}{\|g\|^2} \geq \frac{1}{4} \left(\frac{\int_X |(g^2)'(x)| \, \mathrm{d}x}{\|g\|^2} \right)^2 \tag{6.2}$$

where we used Cauchy-Schwarz for the latter inequality. Setting $X(t) := \{ x \in X \mid g(x)^2 > t \}$, the co-area formula and Fubini yield

$$\frac{\int_X |(g^2)'(x)| \, \mathrm{d}x}{\|g\|^2} = \frac{\int_0^\infty |\{ x \in X \mid g(x)^2 = t \}| \, \mathrm{d}t}{\int_0^\infty \mathrm{vol}_1 X(t) \, \mathrm{d}t} \geq \frac{\int_0^{t_0} |\partial X(t)| \, \mathrm{d}t}{\int_0^{t_0} \mathrm{vol}_1 X(t) \, \mathrm{d}t}$$

since $\{g^2 = t\} \supset \partial X(t)$. Here, $t_0 := \max g(X)^2 > 0$ because $X_+ \neq \emptyset$. Moreover, $X(t)$ is open (g is continuous), $\mathrm{vol}_1 X(t) \leq \mathrm{vol}_1 X_+ \leq \mathrm{vol}_1 X_+^{\mathrm{c}} \leq \mathrm{vol}_1 X(t)^{\mathrm{c}}$, $X(t) \neq \emptyset$ for $t \in [0, t_0)$ and $X(t) \neq X$ for all $t \geq 0$ since $X_+ \neq X$. The definition of Cheeger's constant finally yields the lower bound $h(X)$ for the last fraction. □

Remark 6.2. One might ask whether similar results hold for more general boundary spaces $\mathscr{G}$ (i.e., the metric graph Laplacian $\Delta_{\mathscr{G}}$). There are several problems in the general case:

- If the projection P_v associated to $\mathscr{G}_v$ has complex entries, the eigenfunction may no longer be chosen to be real-valued.
- If the function $f \in \mathrm{dom}\, \Delta_{\mathscr{G}}$ is not continuous at a vertex, (e.g., negative on one edge and positive on another edge meeting in the same vertex), the boundary terms of g appearing from partial integration in (6.2) may not vanish at this vertex.
- The eigenfunction associated to the first non-zero eigenvalue may not change its sign (e.g., if it is a Dirichlet function on a single edge). In this case, one needs a modified Cheeger constant (with $\mathrm{vol}_1 Y$ in the denominator, and $Y \subset X$ open, not intersecting the "Dirichlet" vertices.

Cheeger's theorem for a (standard) finite discrete graph $G = (V, E, \partial)$ can be proven in a similar way. For simplicity, we assume that all weights are the same, say $\ell_e = 1$, and that the graph has no self-loops. We define Cheeger's constant for the discrete graph G as

$$h(G) := \inf_W \frac{|E(W, W^c)|}{\min(\mathrm{vol}_0 W, \mathrm{vol}_0 W^c)}, \tag{6.3}$$

where the infimum runs over all subsets $W \subset V$ such that $W \neq \emptyset$ and $W \neq V$. Furthermore, $E(W, W^c)$ is the set of all edges having one vertex in W and the other one in W^c. The volume of W is defined as $\mathrm{vol}_0 W := \sum_{v \in W} \deg w$. Note that $\mathrm{vol}_0 W = \|\mathbb{1}_W\|^2_{\ell_2(V)}$ (see (2.4)). For a proof of the next theorem, see e.g. [Ch97, Thm. 2.2].

Theorem 6.3. *Assume that G is a connected, finite discrete graph with standard vertex space $\mathscr{G}^{\mathrm{std}}$ and denote by $\lambda_2(G) > 0$ the first non-zero eigenvalue of the standard discrete graph Laplacian as defined in (2.2). Then we have*

$$\lambda_2(G) \geq \frac{h(G)^2}{2}.$$

Again, it would be interesting to carry over the above result for more general discrete Laplacians, namely for $\mathbf{\Delta}_{\mathscr{G}}$ and a general vertex space $\mathscr{G}$ associated to G.

Let us finally mention an upper bound on the second eigenvalue in terms of the distance of subsets (see [FT04b] or [CGY96] for the general scheme and a similar result for discrete graphs):

Theorem 6.4. *Let X be a connected, compact metric graph and denote by $\lambda_2(X)$ the second (first non-zero) eigenvalue of the standard metric graph Laplacian on X. Then*

$$\lambda_2(X) \leq \frac{4}{d(A,B)^2} \left(\log \frac{\mathrm{vol}_1 X}{(\mathrm{vol}_1 A \, \mathrm{vol}_1 B)^{1/2}} \right)^2$$

for any two disjoint measurable subsets A, B of X, where $d(A, B)$ denotes the distance between the sets A and B in the metric graph X.

One can prove similar results also for higher eigenvalues. Note that Theorems 6.1 and 6.4 also hold in the manifold case (with the appropriate measures), and that they are consistent with the eigenvalue approximation result of (5.7).

7. Trace formulas

In this last section we present some results concerning the trace of the heat operator. Trace formulas for metric graph Laplacians appeared first in an article of Roth [R84] (see also [Ku07]), where he used standard (Kirchhoff) boundary conditions; more general self-adjoint vertex conditions (energy-independent, see Remark 3.11 (ii)) are treated in [KoS06, KPS07].

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. A *combinatorial path* in the discrete graph G is a sequence $c = (e_0, v_0, e_1, v_1, \ldots, e_n, v_n, e_{n+1})$ where $v_i \in \partial e_i \cap \partial e_{i+1}$ for $i = 0, \ldots, n$. We call $|c| := n + 1$ the *combinatorial length* of the path c, 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 $\partial_- c \neq \partial_+ c$. Denote by C_n the set of all properly closed paths of combinatorial length n, 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 $c = (v_0, \ldots, v_n)$ of vertices passed by. In particular, $|C_0| = |V|$, $|C_1| = 0$ (no self-loops) and $|C_2| = 2|E|$. Moreover, $C_3 = \emptyset$ is equivalent that G is bipartite. A graph G is called *bipartite*, if $V = V_+ \cup V_-$ with $E = E(V_+, V_-)$, see Eq. (6.3).

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 $\gamma\colon [0,1] \longrightarrow X$ be a *metric path* in the metric graph X, 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 $\gamma(t) \in X^1 = X \setminus V$, i.e., inside an edge. In particular, a path in X cannot turn its direction inside an edge. We denote the set of all paths from x to y by $\Gamma(x,y)$.

Associated to a metric path $\gamma \in \Gamma(x,y)$ there is a unique combinatorial path $c_\gamma = (e_0, v_0, e_1, v_1, \dots, e_{n-1}, v_n, e_{n+1})$ 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., $x \in \overline{e}_-(c)$, $y \in \overline{e}_+(c)$, 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 (or its closure), and x_e, $y_e \in \overline{I}_e$ are the corresponding coordinates ($x = \Phi_e x_e$, cf. Remark 3.2 (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 this definition is well-defined.

Finally, we need to define the *scattering amplitudes* associated to a combinatorial path $c = (e_0, v_0, \dots, e_n, v_n, e_{n+1})$ and a vertex space $\mathscr{G}$. Denote by $P = \oplus P_v$ its orthogonal projection in $\mathscr{G}^{\max}$ onto $\mathscr{G}$. Denote by $S := 2P - \mathbb{1}$ the corresponding scattering matrix defined in Eq. (3.3). In particular, S is local, i.e., $S = \oplus_v S_v$ and we define

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

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 $\mathscr{G}^{\mathrm{std}}$ 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

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

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 metric graph with Laplacian $\Delta_{\mathscr{G}}$ (cf. [R84, Thm. 1], [KPS07, Thm. 4.1]):

Theorem 7.5. *Assume that X is a compact metric graph (without self-loops), $\mathscr{G}$ a vertex space and $\Delta_{\mathscr{G}}$ the associated self-adjoint Laplacian (cf. Proposition 3.8). Then we have*

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

for $t > 0$, where $\operatorname{vol}_1 X = \sum_e \ell_e$ is the total length of the metric graph X.

Remark 7.6.

(i) The first term in the RHS is the term expected from the Weyl asymptotics. The second term is precisely $1/2$ of the index $\operatorname{ind}(X, \mathscr{G})$ of the metric (or discrete) graph X with vertex space $\mathscr{G}$, i.e., the Fredholm index of $\mathrm{d}_{\mathscr{G}}$. In Theorem 4.3 we showed that the index is the same as the discrete index $\operatorname{ind}(G, \mathscr{G})$ (the Fredholm index of $\mathsf{d}_{\mathscr{G})}$). In [KPS07], the authors calculated the second term as $(\operatorname{tr} S)/4$, but since $S = 2P - \mathbb{1}$, we have $\operatorname{tr} S = 2\dim\mathscr{G} - \dim\mathscr{G}^{\max} = 2(\dim\mathscr{G} - |E|)$. The last term in the trace formula comes from an combinatorial expansion.

(ii) The sum over prime cycles of the metric graph X 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, Ku07, KuN05] showed that if X does not have self-loops and 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 [KPS07]. Counterexamples in [R84, GS01, BSS06] show that the rational independence is really needed, i.e., 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 closure of the same edge (and not both on opposite sides of ∂e) and 0 otherwise. The trace of $\mathrm{e}^{-t\Delta_{\mathscr{G}}}$ 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 [KPS07].

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, and that all lengths are the same ($\ell_e = 1$). For simplicity, we write $v \sim w$ if v, w are connected by an edge. Let $\mathscr{G}$ be an associated vertex space. Since $\Delta_{\mathscr{G}} = \mathbb{1} - M_{\mathscr{G}}$ and $M_{\mathscr{G}}$ (see Eq. (2.7)) are bounded operators on $\mathscr{G}$, we have

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

Furthermore, using (2.7) n-times, we obtain

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

and

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

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

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

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*

$$\operatorname{tr} \mathrm{e}^{-t\Delta_{\mathscr{G}}} = \mathrm{e}^{-t} \sum_{n=0}^{\infty} \sum_{c \in C_n} \frac{t^n}{n!} W_{\mathscr{G}}(c) = \mathrm{e}^{-t} \sum_{c \in C} \frac{t^{|c|}}{|c|!} W_{\mathscr{G}}(c). \tag{7.1}$$

Let us interprete the weight in the standard case $\mathscr{G} = \mathscr{G}^{\mathrm{std}}$. Here, $A_{\mathscr{G}^{\mathrm{std}}}(v, w)$ can be interpreted as operator from $\mathbb{C}(\deg w)$ to $\mathbb{C}(\deg v)$ (the degree indicating the corresponding ℓ_2-weight) with $A_{\mathscr{G}^{\mathrm{std}}}(v, w) = 1$ if v, w are connected and 0 otherwise. Viewed as multiplication in $\mathbb{C}$ (without weight), $A_{\mathscr{G}^{\mathrm{std}}}(v, w)$ is unitarily equivalent to the multiplication with $(\deg v \deg w)^{-1/2}$ if $v \sim w$ resp. 0 otherwise. In particular, if $c = (v_0, \ldots, v_{n-1})$ 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 (7.1) reads as

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

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" $W_{\mathscr{G}}(c)$ for general vertex spaces.

References

[BaF06] M. Baker and X. W. C. Faber, *Metrized graphs, Laplacian operators, and electrical networks*, Quantum graphs and their applications, Contemp. Math., vol. 415, Amer. Math. Soc., Providence, RI, 2006, pp. 15–33.

[BaR07] M. Baker and R. Rumely, *Harmonic analysis on metrized graphs*, Canad. J. Math. **59** (2007), no. 2, 225–275.

[BSS06] R. Band, T. Shapira, and U. Smilansky, *Nodal domains on isospectral quantum graphs: the resolution of isospectrality?*, J. Phys. A **39** (2006), 13999–14014.

[vB85] J. von Below, *A characteristic equation associated to an eigenvalue problem on C^2-networks*, Linear Algebra Appl. **71** (1985), 309–325.

[BGP08] J. Brüning, V. Geyler, and K. Pankrashkin, *Spectra of self-adjoint extensions and applications to solvable Schrödinger operators*, Rev. Math. Phys. **20** (2008), 1–70.

[BL92] J. Brüning and M. Lesch, *Hilbert complexes*, J. Funct. Anal. **108** (1992), no. 1, 88–132.

[CaW05] D. I. Cartwright and W. Woess, *The spectrum of the averaging operator on a network (metric graph)*, to appear in Illinois J. Math, `arXiv:math/0509595` (2005).

[C97] C. Cattaneo, *The spectrum of the continuous Laplacian on a graph*, Monatsh. Math. **124** (1997), no. 3, 215–235.

[CdV98] Y. Colin de Verdière, *Spectres de graphes*, Cours Spécialisés [Specialized Courses], vol. 4, Société Mathématique de France, Paris, 1998.

[CGY96] F. R. K. Chung, A. Grigor′yan, and S.-T. Yau, *Upper bounds for eigenvalues of the discrete and continuous Laplace operators*, Adv. Math. **117** (1996), no. 2, 165–178.

[Ch97] F. R. K. Chung, *Spectral graph theory*, CBMS Regional Conference Series in Mathematics, vol. 92, Washington, DC, 1997.

[D84] J. Dodziuk, *Difference equations, isoperimetric inequality and transience of certain random walks*, Trans. Amer. Math. Soc. **284** (1984), no. 2, 787–794.
[EP07] P. Exner and O. Post, *Quantum networks modelled by graphs*, Preprint `arXiv:0706.0481` (2007).
[F06] X. W. C. Faber, *Spectral convergence of the discrete Laplacian on models of a metrized graph*, New York J. Math. **12** (2006), 97–121.
[FT04a] J. Friedman and J.-P. Tillich, *Calculus on graphs*, Preprint `arXiv:cs.DM/0408028` (2004).
[FT04b] ———, *Wave equations for graphs and the edge-based Laplacian*, Pacific J. Math. **216** (2004), no. 2, 229–266.
[FKW07] S. Fulling, P. Kuchment, and J. H. Wilson, *Index theorems for quantum graphs*, J. Phys. A **40** (2007), no. 47, 14165–14180.
[Gr07] D. Grieser, *Spectra of graph neighborhoods and scattering*, Preprint (2007).
[GS01] B. Gutkin and U. Smilansky, *Can one hear the shape of a graph?*, J. Phys. A **34** (2001), no. 31, 6061–6068.
[Ha00] M. Harmer, *Hermitian symplectic geometry and extension theory*, J. Phys. A **33** (2000), no. 50, 9193–9203.
[HP06] P. Hislop and O. Post, *Exponential localization for radial random quantum trees*, Preprint (math-ph/0611022) (2006).
[HSh99] Y. Higuchi and T. Shirai, *A remark on the spectrum of magnetic Laplacianon a graph*, Yokohama Math. J. **47** (1999), 129–141.
[HSh04] ———, *Some spectral and geometric properties for infinite graphs*, Discrete geometric analysis, Contemp. Math., vol. 347, Amer. Math. Soc., Providence, RI, 2004, pp. 29–56.
[KPS07] V. Kostrykin, J. Potthoff, and R. Schrader, *Heat kernels on metric graphs and a trace formula*, Preprint math-ph/0701009 (2007).
[KoS99] V. Kostrykin and R. Schrader, *Kirchhoff's rule for quantum wires*, J. Phys. A **32** (1999), no. 4, 595–630.
[KoS03] ———, *Quantum wires with magnetic fluxes*, Comm. Math. Phys. **237** (2003), no. 1-2, 161–179, Dedicated to Rudolf Haag.
[KoS06] ———, *Laplacians on metric graphs: eigenvalues, resolvents and semigroups*, Quantum graphs and their applications, Contemp. Math., vol. 415, Amer. Math. Soc., Providence, RI, 2006, pp. 201–225.
[K04] P. Kuchment, *Quantum graphs: I. Some basic structures*, Waves Random Media **14** (2004), S107–S128.
[K05] ———, *Quantum graphs. II. Some spectral properties of quantum and combinatorial graphs*, J. Phys. A **38** (2005), no. 22, 4887–4900.
[KuN05] P. Kurasov and M. Nowaczyk, *Inverse spectral problem for quantum graphs*, J. Phys. A **38** (2005), no. 22, 4901–4915.
[Ku07] P. Kurasov, *Graph Laplacians and topology*, Ark. Mat. (to appear).
[L02] W. Lück, *L^2-invariants: theory and applications to geometry and K-theory*, Ergebnisse der Mathematik und ihrer Grenzgebiete., vol. 44, Springer-Verlag, Berlin, 2002.
[MW89] B. Mohar and W. Woess, *A survey on spectra of infinite graphs*, Bull. London Math. Soc. **21** (1989), no. 3, 209–234.
[N87] S. Nicaise, *Spectre des réseaux topologiques finis*, Bull. Sci. Math. (2) **111** (1987), no. 4, 401–413.
[Pa06] K. Pankrashkin, *Spectra of Schrödinger operators on equilateral quantum graphs*, Lett. Math. Phys. **77** (2006), no. 2, 139–154.
[Pa07] ———, *Reduction of quantum graphs to tight-binding Hamiltonians*, talk at the Isaac Newton Institute (INI), Cambridge(03-04-2007).
[P06] O. Post, *Spectral convergence of quasi-one-dimensional spaces*, Ann. Henri Poincaré **7** (2006), no. 5, 933–973.
[P07a] ———, *Equilateral quantum graphs and boundary triples*, Preprint `arXiv:0712.1501` (2007).
[P07b] ———, *First order approach and index theorems for discrete and metric graphs*, Preprint `arXiv:0708.3707` (2007).
[R84] J.-P. Roth, *Le spectre du laplacien sur un graphe*, Théorie du potentiel (Orsay, 1983), Lecture Notes in Math., vol. 1096, Springer, Berlin, 1984, pp. 521–539.
[Sh00] T. Shirai, *The spectrum of infinite regular line graphs*, Trans. Amer. Math. Soc. **352** (2000), no. 1, 115–132.
[So04] M. Solomyak, *On the spectrum of the Laplacian on regular metric trees*, Waves Random Media **14** (2004), no. 1, S155–S171, Special section on quantum graphs.

Institut für Mathematik, Humboldt-Universität zu Berlin, Rudower Chaussee 25, 12489 Berlin, Germany

E-mail address: `post@math.hu-berlin.de`