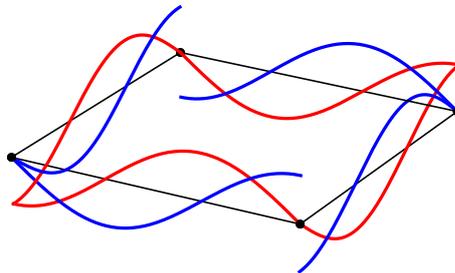


Bachelor thesis

**Spectral comparison of the standard Laplacian
on equilateral finite metric graphs subjected to
Kirchhoff and Anti-Kirchhoff vertex conditions**

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Abstract

Quantum graphs are metric graphs that are equipped with a differential operator acting on the edges of the graph, alongside with a set of meaningful vertex conditions. Structures like these often arise as simplified models in mathematical physics when considering the propagation of waves in wire-like configurations. From the various different kinds of quantum graphs, in this work, only two types are being considered. The focus is set upon equilateral finite quantum graphs equipped with the negative second derivative as their differential operator. For the vertex conditions it will be distinguished between the natural Kirchhoff conditions on one hand, and the so-called Anti-Kirchhoff conditions on the other. Both types of quantum graphs will be analyzed with respect to the spectrum of the associated differential operator. Since the two vertex conditions can be considered to be dual to each other, one might wonder if and how the spectra of the respective operators are related. The answer will be presented in three steps. At first a qualitative description for both spectra is derived, which will culminate in the main intermediate result stating that both spectra are discrete subsets of the nonnegative real numbers. As a second step a quantitative spectral analysis is conducted, taking into account the underlying graph structure. Finally, as the third and last step, the obtained results will be used to compare both of the spectra, and illustrate this comparison by means of four generic quantum graphs with different adjacency properties.

1 Introduction

This work presents a small excerpt from the spectral theory of differential operators associated with so-called quantum graphs. The notion of a quantum graph refers to a graph-like structure of finitely or infinitely many vertices, connected by edges which are identified with one dimensional intervals. The quantum graph transcends this metric substructure by being additionally equipped with a differential operator that acts on a direct sum of function spaces each of which is defined on one of the edge-intervals of the graph. Finally, the communication between functions acting on adjacent edges is controlled by a set of vertex conditions. These conditions, which are the analogous notions to the boundary conditions in boundary value problems of ordinary or partial differential equations, state constraints for edge-functions whose domain overlaps at common vertices.

Structures like quantum graphs have appeared in scientific works for the first time in the 1930s in the context of chemistry where they were used to model the motion of electrons between atoms, see for example [Pau36]. Since then numerous other application in various research areas like physics, chemistry, biology, engineering and pure mathematics have emerged - and are still emerging - making the respective literature on quantum graphs immensely rich. We refer to the survey paper [Kuc02] which provides a detailed overview of different applications with emphasis on spectral problems and to [Kuc04] which contains over 700 references.

As it has been stated above - and as one would expect when confronted with the overwhelming amount of research articles in this field - we will only treat a small subset of possible types of quantum graphs here. The focus will be set on equilateral and finite quantum graphs, with the standard Laplacian acting as a differential operator, subjected to either Kirchhoff or Anti-Kirchhoff conditions. The term equilateral refers to the length of the edges of the quantum graphs, stating that we assume them all to be of the same length. Also we will only consider graphs with finitely many vertices, and hence finitely many edges. By these assumptions we omit any effects coming from the varying edge lengths in the graph and instead emphasize the pure adjacency structure. Also we do not include issues arising from graphs with infinitely many edges. The standard Laplacian, that is the negative second derivative acting on each edge as on a conventional interval, is the simplest elliptic differential operator. More general differential operators like the Schrödinger or magnetic Schrödinger operator will not be part of the discussion. Finally a word on the vertex conditions. The natural Kirchhoff conditions, sometimes also called δ -type or even Neumann-conditions, demand continuity of the edge-functions whose domains overlap at a shared vertex combined with a so-called flow conditions stating that the outgoing derivatives at each edge should sum up to zero. The Anti-Kirchhoff conditions, also called δ' -type conditions, are much less common than the Kirchhoff ones. They are in some respect dual to the aforementioned ones, since they flip the conditions between the derivatives and values resulting in a continuity-condition for the derivatives and a “flow”-condition for the function values at the vertices.

We will analyze the spectra of the operators associated with these two types of quantum graphs. Since both types only differ in their vertex conditions, which are - as mentioned above - in some sense dual, and hence related to each other, one might wonder if this relationship will also be reflected in the operator spectra. To answer this question we will take a three-step approach. As our first step we will analyze the spectrum of both graphs qualitatively. Our results will show that both spectra are real, nonnegative and discrete. On our way to this intermediate result we will need several results from the theory of unbounded linear operators on Hilbert spaces including the respective spectral theory, which will be provided in Section 2. We are going to use these results to show that both operators associated with the considered quantum graphs are self-adjoint and nonnegative. For the discreteness of the spectrum we will utilize one of the Sobolev-embedding theorems showing that the resolvents of the operators are compact. All these results are given in Section 3.2.1. As the second step we will perform a quantitative analysis of the spectra in Section 3.2.2. For that purpose we will apply the so-called adjacency calculus introduced by von Below in [vB84], in which we will transform the eigenvalue-problem to an equivalent matrix eigenvalue-problem. As a third and last step we will use our results from the previous steps to compare the spectra, and illustrate the results for four generic examples, including some plots for the corresponding eigenfunctions. This final step is presented in Section 3.2.4 and 3.2.5.

2 Foundations

2.1 Spectral theory of unbounded operators

In this section, as in the thesis in general, we only consider linear operators on *complex* Hilbert spaces, meaning that all operators in the following are of the same type $T : H \supset \text{dom}(T) \rightarrow H$ with H being a complex Hilbert space.

2.1.1 First notions and the Spectral Mapping Theorem

In operator theory one generally distinguishes between bounded and unbounded linear operators. While in the first case we can always find a constant $M > 0$ such that $\|Tx\| \leq M\|x\|$ for all $x \in H$, such a constant does not exist in the unbounded case. Typical representatives for the unbounded kind are differential operators, which will also play the central role in this work. The notion of an unbounded linear operator is introduced in the following frame, cf. [Wer11, Definition VII.2.1].

Definition 2.1 (Linear Operator). *A linear mapping $T : H \supset \text{dom}(T) \rightarrow H$ whose domain $\text{dom}(T)$ is a subspace of H is called a (linear) operator. We say that T is densely defined if $\text{dom}(T) = H$. An operator $S : H \supset \text{dom}(S) \rightarrow H$ is called an extension of T if $\text{dom}(T) \subset \text{dom}(S)$ and $Sx = Tx$ for all $x \in \text{dom}(T)$. In this case we write $T \subset S$.*

Since all operators in this work are linear, we will usually drop this specification in the following and simply refer to them as operators. Although the above definition also includes bounded operators it is usually introduced in the context of unbounded operators, since we normally have $\text{dom}(T) = H$ in the bounded case. In other words: for an unbounded operator T one frequently has $\text{dom}(T) \subsetneq H$ which motivates Definition 2.1.

The goal of the subsequent considerations is to give a short introduction in the spectral theory of unbounded operators, aiming at results which are important in the framework of spectral analyses of differential operators on compact graphs. Main references have been [Wer11], [AU10], [Bre10], [EN99] and [Are]. More specific citations will be given whenever we refer to important theorems or definitions from these sources.

Since we want to discuss aspects of spectral theory, it makes sense to start with the central notion of this field, that is the spectrum of an operator, alongside with its counterpart, the resolvent set, cf. [Wer11, Definition VII.2.14].

Definition 2.2 (Spectrum and resolvent set). *Let $T : H \supset \text{dom}(T) \rightarrow H$, then we define the resolvent set $\rho(T)$ and the spectrum $\sigma(T)$ of T as*

- (i) $\rho(T) := \{\lambda \in \mathbb{C} : (\lambda - T) : \text{dom}(T) \rightarrow H \text{ is bijective and } (\lambda - T)^{-1} \in \mathcal{L}(H)\}$
- (ii) $\sigma(T) := \mathbb{C} \setminus \rho(T)$.

As customary, we refer with $\mathcal{L}(H)$ to the set of bounded linear operators on H . Essential for the definition of the spectrum is that the operator $(\lambda - T)^{-1}$ is not only exists, but that this inverse is additionally bounded.

We see that an element of $\rho(T)$ is always associated with a bounded linear operator, which leads to the following definition, see [Wer11, Definition VII.2.14].

Definition 2.3 (Resolvent operator). *Let $T : H \supset \text{dom}(T) \rightarrow H$. If $\lambda \in \rho(T)$ we define the resolvent operator of T at λ as $R(\lambda, T) : H \rightarrow \text{dom}(T) \subset H$ as*

$$R(\lambda, T) := (\lambda - T)^{-1}.$$

In the bounded case, that is $T \in \mathcal{L}(H)$, we know that $\sigma(T)$ is a nonempty, compact set in the complex plane (see Proposition A.4). This is a result arising from bounded operators being continuous. Unbounded operators, however, are not continuous, which results in $\sigma(T)$ not necessarily being compact. A somewhat weaker notion than continuity, which takes its place in the spectral theory of unbounded operators, is closedness. The importance of this concept is illustrated by the result that we have $\sigma(T) = \mathbb{C}$ whenever T is not closed [Wer11, p. 354]. In the following we therefore usually assume that the considered operators are closed.

The elements of the spectrum can be categorized according to the properties of $\lambda - T$ and $(\lambda - T)^{-1}$ respectively. One important group are the so-called eigenvalues, which are the elements of the point spectrum, introduced by the following definition, cf. [EN99, Definition 1.6].

Definition 2.4 (Point spectrum). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be closed. If $(\lambda - T) : \text{dom}(T) \rightarrow H$ is not injective for some $\lambda \in \mathbb{C}$, we call λ an eigenvalue of T . We define the point spectrum $\sigma_p(T)$ of T as the set of all its eigenvalues, hence*

$$\sigma_p(T) := \{\lambda \in \mathbb{C} : (\lambda - T) \text{ is not injective}\}.$$

The resolvent operators associated with the elements of the spectrum $\sigma(T)$ are bounded operators. We can hence apply classic results from spectral theory of bounded operators. This usually makes it easier to treat the spectra of the resolvent operators than the spectrum of the considered unbounded operator T . Fortunately, it turns out that both spectra are related to each other. This is the content of the following important result, which can be found in [EN99, Theorem 1.13].

Theorem 2.5 (Spectral Mapping Theorem). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be closed with $\rho(T) \neq \emptyset$ and $\lambda \in \rho(T)$. Then*

$$\begin{aligned} \sigma(R(\lambda, T)) \setminus \{0\} &= (\lambda - \sigma(T))^{-1} := \{(\lambda - \mu)^{-1} \in \mathbb{C} : \mu \in \sigma(T)\} \\ \sigma_p(R(\lambda, T)) \setminus \{0\} &= (\lambda - \sigma_p(T))^{-1} := \{(\lambda - \mu)^{-1} \in \mathbb{C} : \mu \in \sigma_p(T)\}. \end{aligned}$$

Proof. Let $\mu \neq 0$ and $\lambda \in \rho(T)$, then we obtain

$$\begin{aligned} (\mu - R(\lambda, T))x &= \mu(\lambda - \mu^{-1} - T)R(\lambda, T)x && \text{for all } x \in H \\ &= \mu R(\lambda, T)(\lambda - \mu^{-1} - T)x && \text{for all } x \in \text{dom}(T). \end{aligned}$$

This implies the two identities

$$\begin{aligned} \ker(\mu - R(\lambda, T)) &= \ker(\lambda - \mu^{-1} - T) \\ \text{ran}(\mu - R(\lambda, T)) &= \text{ran}(\lambda - \mu^{-1} - T) \end{aligned}$$

from which we conclude that $\tilde{\mu} \in \sigma(R(\lambda, T))$ if and only if $\lambda - \tilde{\mu}^{-1} \in \sigma(T)$. When we only consider the first identity we see that the same also holds for the point spectrum. If we now set $\mu := \lambda - \tilde{\mu}^{-1}$, hence $\tilde{\mu} = (\lambda - \mu)^{-1}$ we arrive at the assertion. \square

The Spectral Mapping Theorem allows us to analyze the spectrum of an operator by using the spectral properties of the resolvent operators. A specific case we are interested in, is when an unbounded operator has a compact resolvent for some $\lambda \in \rho(T)$. In this case it follows that $R(\lambda, T)$ is compact for all $\lambda \in \rho(T)$. This is an immediate consequence from the resolvent identity (Proposition A.8) and the ideal property of compact operators in $\mathcal{L}(H)$, i.e., for $K \in \mathcal{K}(H)$ (where $\mathcal{K}(H)$ denotes the set of compact operators on H) and $S \in \mathcal{L}(H)$ it follows $KS, SK \in \mathcal{K}(H)$. Consequently it makes sense to introduce the following definition, cf. [Are, Definition 1.3.1].

Definition 2.6 (Operator with compact resolvent). *An operator $T : H \supset \text{dom}(T) \rightarrow H$ with $\rho(T) \neq \emptyset$ is said to have compact resolvent if there exists $\lambda \in \rho(T)$ such that $R(\lambda, T)$ is compact.*

The next lemma provides us with a criterion to check whether an operator has compact resolvent or not, which is quite useful for our applications, cf. [Are, p. 8].

Lemma 2.7 (Criterion for compact resolvent). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be an operator with $\rho(T) \neq \emptyset$. Then T has compact resolvent if and only if the embedding $(\text{dom}(T), \|\cdot\|_T) \hookrightarrow H$, where $\|\cdot\|_T$ denotes the graph norm, is compact.*

Proof. First, assume that T has compact resolvent, and consider $\lambda \in \rho(T) \neq \emptyset$. Recalling that $T : (\text{dom}(T), \|\cdot\|_T) \rightarrow H$ is continuous, we conclude that $(\lambda - T)^{-1}(\lambda - T) : (\text{dom}(T), \|\cdot\|_T) \rightarrow H$ is compact as the composition of a continuous and a compact operator, hence $(\text{dom}(T), \|\cdot\|_T) \hookrightarrow H$ is compact. For the converse implication assume that $(\text{dom}(T), \|\cdot\|_T) \hookrightarrow H$ is compact, which we can express by saying that the injection $i : (\text{dom}(T), \|\cdot\|_T) \rightarrow H$ is compact. By the closed graph theorem $(\lambda - T)^{-1} : H \rightarrow (\text{dom}(T), \|\cdot\|_T)$ is continuous, implying that $i(\lambda - T)^{-1} : H \rightarrow H$ is compact as the composition of a continuous and a compact operator. Hence T has compact resolvent, which concludes the proof. \square

Using the Spectral Mapping Theorem 2.5 and the spectral properties of compact operators, see Proposition A.5, we obtain a spectral classification for (unbounded) operators with compact resolvent, see [Are, Prop. 1.3.3].

Corollary 2.8 (Spectrum of operators with compact resolvent). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be an operator with compact resolvent. Then the following holds.*

- (i) T has a pure point spectrum, that is $\sigma(T) = \sigma_p(T)$.
- (ii) The spectrum $\sigma(T)$ is either finite or the spectrum can be expressed as

$$\sigma(T) = \{\lambda_n \in \mathbb{C} : n \in \mathbb{N}\} \quad \text{with} \quad \lim |\lambda_n| = \infty.$$

- (iii) All eigenvalues have finite multiplicity, that is $\dim \ker(\lambda - T) < \infty$ for all $\lambda \in \mathbb{C}$.

2.1.2 The spectrum of self-adjoint operators

From now on we will focus our attention on self-adjoint operators, which is justified by the fact, that all differential operators associated with compact quantum graphs we will encounter later, turn out to be self-adjoint. We will begin with introducing the definition of self-adjointness in the unbounded case, developing criteria for this property, and finally analyze the spectra of self-adjoint unbounded operators.

A property that is closely related to self-adjointness is symmetry, which will be formally introduced in the next definition, cf. [Wer11, Definition VII.2.2].

Definition 2.9 (Symmetric operator). *An operator $T : H \supset \text{dom}(T) \rightarrow H$ is called symmetric if $\langle Tx, y \rangle = \langle x, Ty \rangle$ for all $x, y \in \text{dom}(T)$. If additionally $\langle Tx, x \rangle \geq 0$ holds, we say that T is nonnegative.*

Note that the above definition regarding nonnegative operators makes sense, since for symmetric T one always has $\langle Tx, x \rangle \in \mathbb{R}$, as shown in Lemma 2.10.

An interesting property of symmetric operators, which we will need later, is given by the next auxiliary result, see [Wer11, Lemma VII.2.7].

Lemma 2.10. *Let $T : H \supset \text{dom}(T) \rightarrow H$ be symmetric. Then $(\pm i - T) : \text{dom}(T) \rightarrow \text{ran}(\pm i - T)$ is bijective and $(\pm i - T)^{-1} : \text{ran}(\pm i - T) \rightarrow \text{dom}(T)$ is bounded.*

Proof. The symmetry of T implies $\langle Tx, x \rangle \in \mathbb{R}$ for all $x \in \text{dom}(T)$. Indeed, recalling that for all $x, y \in H$ we have $\langle x, y \rangle = \overline{\langle y, x \rangle}$, it follows $\langle Tx, x \rangle = \langle x, Tx \rangle = \overline{\langle Tx, x \rangle}$ and hence $\langle Tx, x \rangle \in \mathbb{R}$. Consequently we have $\text{Re}\langle Tx, ix \rangle = 0$ for all $x \in H$. Using this result we compute

$$\begin{aligned} \|(\pm i - T)x\|^2 &= \|Tx\|^2 + \|x\|^2 \mp 2\text{Re}\langle Tx, ix \rangle \\ &= \|Tx\|^2 + \|x\|^2 \geq \|x\|^2 \end{aligned}$$

which shows that $\ker(\pm i - T) = \{0\}$. This implies that $(\pm i - T) : \text{dom}(T) \rightarrow H$ is injective and that $(\pm i - T) : \text{dom}(T) \rightarrow \text{ran}(\pm i - T)$ is bijective. We conclude that $(\pm i - T)^{-1} : \text{ran}(\pm i - T) \rightarrow \text{dom}(T)$ exists. Finally we see from

$$\|x\| = \|(\pm i - T)(\pm i - T)^{-1}x\| \geq \|(\pm i - T)^{-1}x\|$$

that $(\pm i - T)^{-1} : \text{ran}(\pm i - T) \rightarrow \text{dom}(T)$ is also bounded, which concludes the proof. \square

An operator is called self-adjoint when it is identical with its so-called adjoint operator. The notion of the adjoint operator will be introduced below, see for example [Wer11, Definition VII.2.3].

Definition 2.11 (Adjoint operator). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be densely defined. The adjoint operator $T^* : H \supset \text{dom}(T^*) \rightarrow H$ is defined by*

$$\langle Tx, y \rangle = \langle x, T^*y \rangle \quad \text{for all } x \in \text{dom}(T), y \in \text{dom}(T^*)$$

with the domain $\text{dom}(T^) := \{y \in H : \exists z \in H \text{ with } \langle Tx, y \rangle = \langle x, z \rangle \text{ for all } x \in \text{dom}(T)\}$. In the case $T = T^*$ we say that T is self-adjoint.*

Note that, according to the above definition, we can only discuss self-adjointness of an operator if it is densely defined. Consequently, whenever we assume self-adjointness of an operator, it implies that this operator is densely defined.

It is worth noting, that in the bounded case, self-adjointness and symmetry are identical concepts. This is the assertion of the Hellinger-Toeplitz Theorem, cf. [Wer11, Theorem V.5.5]. From this perspective we can understand self-adjointness, as well as closedness of an operator, as concepts motivated by the theory of unbounded operators. We see, an unbounded densely defined operator that is symmetric is not necessarily self-adjoint (we only have $T \subset T^*$). But a self-adjoint operator is always symmetric.

The first result concerning the spectrum of a self-adjoint operator T , we are going to show, is that $\sigma(T) \neq \emptyset$. This is clear whenever T is bounded, since $\sigma(T) \neq \emptyset$ for all $T \in \mathcal{L}(H)$, see Proposition A.4. But in the general unbounded case, that is when we are not assuming self-adjointness, $\sigma(T) = \emptyset$ is possible [Wer11, p. 354]. However, if we do assume self-adjointness, the spectrum is nonempty also in the unbounded case.

Theorem 2.12 (Nonempty spectrum). *The spectrum of any self-adjoint operator T is nonempty.*

Proof. As we mentioned before, in the bounded case this result follows from Proposition A.4. Thus, let T be an unbounded self-adjoint operator. Assume that the spectrum is empty, that is $\sigma(T) = \emptyset$, then $\rho(T) = \mathbb{C}$ which implies in particular $0 \in \rho(T)$. Consequently it follows that $R(0, T) = (0 - T)^{-1} = -T^{-1}$ and hence T^{-1} exists and is bounded. Assume $\mathbb{C} \ni \mu \neq 0$ then

$$\begin{aligned}\mu - T^{-1} &= (\mu T - \text{Id})T^{-1} \\ &= -\mu(\mu^{-1} - T)T^{-1}.\end{aligned}$$

Since $0, \mu^{-1} \in \rho(T) = \mathbb{C}$ it follows the right hand side is invertible. We compute its inverse as

$$\begin{aligned}(-\mu(\mu^{-1} - T)T^{-1})^{-1} &= -\mu^{-1}T(\mu^{-1} - T)^{-1} \\ &= \mu^{-1}((\mu^{-1} - T) - \mu^{-1})(\mu^{-1} - T)^{-1} \\ &= \mu^{-1}(\text{Id} - \mu^{-1}(\mu^{-1} - T)^{-1})\end{aligned}$$

which is bounded since $\mu^{-1} \in \rho(T) = \mathbb{C}$. This shows that also $\mu - T^{-1}$ is invertible with bounded inverse, which in turn implies that $\sigma(T^{-1}) = \{0\}$ since we just showed that $\mu \in \rho(T^{-1})$ for all $\mu \neq 0$ and according to Proposition A.4 the spectrum of a bounded operator is not empty, hence $\sigma(T^{-1}) \neq \emptyset$. But since T^{-1} is also self-adjoint (see Proposition A.7) this result shows by Proposition A.6 that $\|T^{-1}\| = 0$ which is equivalent with the absurd result $T^{-1} = 0$. We hence conclude that $\sigma(T) \neq \emptyset$. \square

The next spectral property of a self-adjoint unbounded operator T we want to show is that $\sigma(T) \subset \mathbb{R}$. This result is presented in Theorem 2.15. Before we get there, we need some preparation. We begin with some relations between T and its adjoint T^* , cf. [Wer11, Theorem VII.2.4, VII.2.5].

Lemma 2.13. *Let $T : H \supset \text{dom}(T) \rightarrow H$ be densely defined, then*

- (i) T^* is closed.
- (ii) $\ker(\mp i - T^*) = \text{ran}(\pm i - T)^\perp$.
- (iii) If T is closed and symmetric, then $\text{ran}(\pm i - T)$ is closed.

Proof. (i) Since T is densely defined, its adjoint operator T^* is well defined. Consider the sequence $(y_n) \subset \text{dom}(T^*)$ with $y_n \rightarrow y \in H$ and $T^*y_n \rightarrow z \in H$. Using the continuity of the scalar product we obtain

$$\langle Tx, y \rangle = \lim \langle Tx, y_n \rangle = \lim \langle x, T^*y_n \rangle = \langle x, z \rangle$$

which shows that $y \in \text{dom}(T^*)$ with $T^*y = z$, in other words T^* is closed.

(ii) At first we show $\ker(\mp i - T^*) \supset \text{ran}(\pm i - T)^\perp$. To that end let $y \in \text{ran}(\pm i - T)^\perp$, then we have $\langle (\pm i - T)z, y \rangle = 0$ for all $z \in \text{dom}(T) = \text{dom}(\pm i - T)$. We can hence write $z \mapsto \langle (\pm i - T)z, y \rangle = \langle z, 0 \rangle$ from which we see that $y \in \text{dom}(T^*) = \text{dom}(\mp i - T^*) = (\pm i - T)^*$

with $\langle z, (\mp i - T^*)y \rangle = 0$, thus $(\mp i - T^*)y = 0$ which is $y \in \ker(\mp iT^*)$. If we read these arguments in reverse we obtain the proof for the remaining inclusion $\ker(\mp i - T^*) \subset \text{ran}(\pm i - T)^\perp$.

(iii) Since T is symmetric we can use Lemma 2.10 to show that $(\pm i - T) : \text{dom}(T) \rightarrow \text{ran}(\pm i - T)$ is bijective, hence invertible, and $(\pm i - T)^{-1} : \text{ran}(\pm i - T) \rightarrow \text{dom}(T)$ is bounded, that is continuous. Now consider the sequence $(x_n) \subset \text{dom}(T)$ with $(\pm i - T)x_n \rightarrow y \in \text{ran}(\pm i - T)$. Since $((\pm i - T)x_n)$ is convergent it is a Cauchy sequence, from which we conclude with the continuity of $(\pm i - T)^{-1}$ that (x_n) is a Cauchy sequence in $\text{dom}(T)$. This implies that there exists a limit $x := \lim x_n \in H$ and that $Tx_n \rightarrow y \mp ix$. Since T is closed we have $x \in \text{dom}(T)$ and $Tx = y \mp ix$ and hence $y = (\pm i - T)x \in \text{ran}(\pm i - T)$. This shows $\overline{\text{ran}(\pm i - T)} = \text{ran}(\pm i - T)$, i.e., $\text{ran}(\pm i - T)$ is closed. \square

We will use these rather technical results to obtain criteria for the self-adjointness of an operator, that are more convenient than the original Definition 2.11. We refer to [Wer11, Theorem VII.2.9].

Lemma 2.14 (Criteria for self-adjointness). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be symmetric and densely defined, then the following assertions are equivalent.*

- (i) T is self-adjoint.
- (ii) T is closed and $\ker(\pm i - T^*) = \{0\}$.
- (iii) $\text{ran}(\pm i - T) = H$.

Proof. (i) \Rightarrow (ii) From Lemma 2.13 (i) we know that T^* is closed, and since T is self-adjoint, that is $T = T^*$ we see that T is closed too. Using again Lemma 2.13 (i) we know that $(\pm i - T) : \text{dom}(T) \rightarrow H$ is injective, hence $\ker(\pm i - T) = \{0\}$ which implies $\ker(\pm i - T^*) = \{0\}$ with the self-adjointness of T .

(ii) \Rightarrow (iii) Since T is symmetric we can use the second part of Lemma 2.13 to conclude $\text{ran}(\pm i - T)^\perp = \{0\}$. Since T is also assumed to be closed this result in combination with the last part of Lemma 2.13 implies $\text{ran}(\pm i - T) = H$.

(iii) \Rightarrow (i) Since $T \subset T^*$, hence $\text{dom}(T) \subset \text{dom}(T^*)$ we only have to show the inclusion $\text{dom}(T^*) \subset \text{dom}(T)$. In this case T would be a symmetric operator with $\text{dom}(T) = \text{dom}(T^*)$, which implies self-adjointness. Let $y \in \text{dom}(T^*) \subset H$ then according to (iii) we can find an $x \in \text{dom}(T) = \text{dom}(\pm i - T)$ such that $(\pm i - T^*)y = (\pm i - T)x$. Because of $T \subset T^*$ we arrive at $(\pm i - T^*)y = (\pm i - T^*)x$, which implies $y = x \in \text{dom}(T)$ since $(\pm i - T^*)$ is injective according to Lemma 2.13 and (iii). This shows $\text{dom}(T^*) \subset \text{dom}(T)$ and concludes the proof. \square

This already brings us to our central result in this short subsection. With criterion (iii) from Lemma 2.14, which is sometimes called the range condition, we are able to show that the spectrum of a self-adjoint operator is real, cf. [Wer11, Theorem VII.2.16]

Theorem 2.15 (Spectrum of self-adjoint operator). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be a densely defined, symmetric operator. Then T is self-adjoint if and only if $\sigma(T) \subset \mathbb{R}$.*

Proof. The idea of the proof is to show that any non-real $z \in \mathbb{C}$ is included in the resolvent set $\rho(T)$, i.e., $(z - T) : \text{dom}(T) \rightarrow H$ is bijective and $(z - T)^{-1}$ is bounded. To that end we pick $\lambda, \mu \in \mathbb{R}$ with $\mu \neq 0$ such that $z := \lambda + i\mu \in \mathbb{C} \setminus \mathbb{R}$, and consider the auxiliary operator $S : \text{dom}(T) \rightarrow H$ defined as

$$S := \frac{T}{\mu} - \frac{\lambda}{\mu}.$$

It is easy to check that S is symmetric, and that $\text{dom}(S^*) = \text{dom}(T^*) = \text{dom}(S)$, hence that S is self-adjoint. This allows us to use Lemma 2.14 which leads to $\text{ran}(i - S) = H$. We conclude

$$H = \text{ran}(i - S) = \text{ran}(\mu^{-1}(\lambda + i\mu - T)) = \text{ran}(z - T)$$

which shows that $(z - T) : \text{dom}(T) \rightarrow H$ is surjective. To show that $(z - T)$ is also injective, we note that $z - T = \mu(i - S)$. Since S is symmetric we can apply Lemma 2.10 to see that $(i - S)$ and hence $(z - T)$ is injective with $(z - T)^{-1} : H \rightarrow \text{dom}(T)$ being bounded. Summarizing our results we see that $z \in \rho(T)$ which implies $\sigma(T) \subset \mathbb{R}$. For the converse implication, let $\sigma(T) \subset \mathbb{R}$, hence $\pm i \in \rho(T)$ which implies $T \pm i$ being bijective, hence $\text{ran}(\pm i - T) = H$. This shows self-adjointness of T by Proposition 2.14, and concludes the proof. \square

We can further narrow down the spectrum of a self-adjoint operator when it is nonnegative, see Definition 2.9. In this case the spectrum is nonnegative as well.

Lemma 2.16 (Nonnegative spectrum). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be nonnegative and self-adjoint. Then $\sigma(T)$ is contained in $[0, \infty) \subset \mathbb{R}$.*

Proof. Since T is self-adjoint we already know that $\sigma(T) \subset \mathbb{R}$, see Theorem 2.15. Now assume there exists a $\lambda \in \sigma(T)$ with $\lambda < 0$. Then by definition there is an $0 \neq f \in H$ with $Tf = \lambda f$. We hence conclude

$$0 \leq \langle Tf, f \rangle = \langle \lambda f, f \rangle = \lambda \|f\|_H^2 < 0$$

which is absurd. It follows $\lambda \geq 0$ which is the assertion. \square

2.1.3 Symmetric forms associated with operators

Until this point we discussed the spectrum of self-adjoint operators with compact resolvent. With these results we can characterize the spectrum of a given operator as soon as we identified it as being self-adjoint and/or having compact resolvent. Regarding self-adjointness, we already came up with a criterion which can be used to determine whether or not a given operator is self-adjoint or not, that is Lemma 2.14. However, it turns out, that its applications might require some effort.

In this subsection we want to present an approach, based on [Are, Section 3.4], which often makes it easier to check the operator properties. This approach is based on the idea, that a certain type of operator can be associated with a unique bilinear form, which reflects the operator properties, and is usually easier to analyze.

We begin by introducing a new kind of operator, cf. [Are, Definition 1.4.1].

Definition 2.17 (Dissipative operator). *An operator T on H is called dissipative if*

$$\text{Re}\langle Tx, x \rangle \leq 0 \quad \text{for all } x \in \text{dom}(T).$$

In the symmetric case, we have $\langle Tx, x \rangle \in \mathbb{R}$, and can thus write $\langle Tx, x \rangle \leq 0$. With respect to Definition 2.9 we could also call such an operator nonpositive.

It turns out that the spectra of dissipative operators have an interesting property described by the next result, cf. [Are, Proposition 1.4.2].

Proposition 2.18. *Let $T : H \supset \text{dom}(T) \rightarrow H$ be a dissipative operator. Assume there exists some $\lambda \in \mathbb{C}_+ := \{z \in \mathbb{C} : \text{Re}(z) > 0\}$ such that $(\lambda - T)$ is surjective. Then $\mu \in \rho(T)$ with $\|R(\mu, T)\| \leq \text{Re}(\mu)^{-1}$ for all $\mu \in \mathbb{C}_+$.*

Proof. Let $\mu \in \mathbb{C}_+$ such that $(\mu - T)$ is surjective. Now consider $x \in \text{dom}(T)$ and $y := (\mu - T)x \in H$, then one obtains with the dissipativity of T and the Cauchy-Schwarz inequality

$$\begin{aligned} \text{Re}(\mu)\|x\|^2 &= \text{Re}\langle \mu x, x \rangle \\ &= \text{Re}\langle x, y \rangle + \text{Re}\langle Tx, x \rangle \\ &\leq \text{Re}\langle x, y \rangle \\ &\leq \|x\|\|y\| \end{aligned}$$

hence $\text{Re}(\mu)\|x\| \leq \|y\|$. If additionally $\mu \in \rho(T)$, that is $\mu \in \mathbb{C}_+ \cap \rho(T) =: M$ then $y = R(\mu, T)^{-1}x$ and it follows $\|R(\mu, T)\| \leq \text{Re}(\mu)^{-1}$ as claimed. Since $\rho(T)$ and \mathbb{C}_+ are open, M is open too. Also M is closed, which follows from Corollary A.10 and $\|R(\mu, T)\| \leq \text{Re}(\mu)^{-1}$. Since M is nonempty and connected this shows that $M = \mathbb{C}_+$. \square

Dissipative operators are closely related to symmetric operators. This is expressed in the next proposition, cf. [Are, Proposition 1.4.5].

Proposition 2.19. *Let $T : H \supset \text{dom}(T) \rightarrow H$ be an operator, then the following assertions are equivalent.*

- (i) T is symmetric;

(ii) $\langle Tx, x \rangle \in \mathbb{R}$ for all $x \in \text{dom}(T)$;

(iii) $\pm iT$ is dissipative.

Proof. It is easy to see that (ii) and (iii) are equivalent. Indeed, if $\langle Tx, x \rangle \in \mathbb{R} \forall x \in \text{dom}(T)$ it follows that $\text{Re}\langle \pm iTx, x \rangle = \text{Re}\langle \pm i\langle Tx, x \rangle \rangle = 0$ for all $x \in \text{dom}(T)$, which by Definition 2.17 shows dissipativity of $\pm iT$. On the other hand if $\pm iT$ are dissipative and $\langle Tx, x \rangle = \alpha + i\beta$ for some $\beta \in \mathbb{R} \setminus \{0\}$ then $\text{Re}\langle \pm iTx, x \rangle = \text{Re}\langle \pm i\langle Tx, x \rangle \rangle = \mp\beta$ switches sign, hence $\beta = 0$ and thus $\langle Tx, x \rangle \in \mathbb{R}$ for all $x \in \text{dom}(T)$.

It remains to show that (i) and (ii) are equivalent. We begin with (i) \Rightarrow (ii). If T is symmetric then $\langle Tx, x \rangle = \langle x, Tx \rangle = \overline{\langle Tx, x \rangle}$ for all $x \in \text{dom}(T)$ where the second equality results from the properties of the scalar product $\langle \cdot, \cdot \rangle$, hence $\langle Tx, x \rangle \in \mathbb{R}$. To show (ii) \Rightarrow (i) we use the polarization identity, cf. Proposition A.2. Note that due to the symmetry of T by setting $s(x, y) := \langle Tx, y \rangle$ we obtain a sesquilinear form with associated quadratic form $q(x) := \langle Tx, x \rangle$. Applying the polarization identity gives us

$$\begin{aligned} \langle Tx, y \rangle &= \frac{1}{4} \sum_{k=0}^3 i^k \langle T(x + i^k y), x + i^k y \rangle \\ &= \frac{1}{4} \sum_{k=0}^3 i^k \langle T((-i)^k x + y), (-i)^k x + y \rangle \\ &= \overline{\langle Ty, x \rangle} = \langle x, Ty \rangle. \end{aligned}$$

□

The last two results allow us to characterize the spectrum of symmetric operators. Interestingly, this type of operator only allows four possible forms, cf. [Are, Proposition 1.4.6].

Proposition 2.20. *Let $T : H \supset \text{dom}(T) \rightarrow H$ be a symmetric operator, then $\sigma(T)$ has one of the following forms.*

(i) $\sigma(T) = \mathbb{C}$

(ii) $\sigma(T) = \{z \in \mathbb{C} : \text{Im}(z) \geq 0\}$

(iii) $\sigma(T) = \{z \in \mathbb{C} : \text{Im}(z) \leq 0\}$

(iv) $\sigma(T) \subset \mathbb{R}$

Proof. Since T is symmetric, iT is dissipative according to Proposition 2.19. Now assume that $\mu \in \rho(iT)$ with $\text{Re}(\mu) > 0$, then $(\mu - iT) = i(-i\mu - T)$ is surjective, that is $-i\mu \in \rho(T)$ with $\text{Im}(-i\mu) < 0$. Now we use Proposition 2.18 to see that $\rho(T) \subset \{z \in \mathbb{C} : \text{Im}(z) < 0\}$. Similar arguments show that when $\text{Re}(\mu) < 0$ it follows $\rho(T) \subset \{z \in \mathbb{C} : \text{Im}(z) > 0\}$. Considering all combinations of these two cases, recalling that $\sigma(T) = \mathbb{C} \setminus \rho(T)$ we obtain the four possibilities that are stated in the assertion. □

We use this information on symmetric operators to deduce a criterion for dissipative and self-adjoint operators, cf [Are, p. 13].

Proposition 2.21. *A densely defined operator $T : H \supset \text{dom}(T) \rightarrow H$ is dissipative and self-adjoint if and only if the following conditions hold.*

(i) T is symmetric;

(ii) $\langle Tx, x \rangle \leq 0$ for all $x \in \text{dom}(T)$;

(iii) $(\text{Id} - T)$ is surjective.

Proof. If T is dissipative and self-adjoint, then T is especially symmetric, hence $\langle Tx, x \rangle \in \mathbb{R}$ for all $x \in \text{dom}(T)$ and due to dissipativity it follows $\langle Tx, x \rangle \leq 0 \forall x \in \text{dom}(T)$. Now assume $1 \in \sigma(T)$, that is $Tx = x$ for some $0 \neq x \in H$, then $\langle Tx, x \rangle = \langle x, x \rangle = \|x\|^2 > 0$ which contradicts dissipativity. Hence $1 \in \rho(T)$ which implies that $(\text{Id} - T)$ is surjective. On the other hand, if (i), (ii) and (iii) hold we refer to Proposition 2.20 to see that $\sigma(T) \subset \mathbb{R}$ (note that $1 \in \rho(T)$), which according to Proposition 2.15 implies that T is self-adjoint. Finally dissipativity is given by (ii), concluding the proof. □

We will use this criterion to develop the notion of a sesquilinear form that is associated with a dissipative and self-adjoint operator. This will allow us to analyze the properties of the given operator by analyzing its associated form.

We begin with introducing some vocabulary, cf. [Are, p. 40, 41].

Definition 2.22 (Sesquilinear form). *Let V be a complex vector space, then a mapping of the kind $a : V \times V \rightarrow \mathbb{C}$ is called a sesquilinear form on V if it satisfies the following conditions.*

$$\begin{aligned} a(x_1 + x_2, y) &= a(x_1, y) + a(x_2, y) \\ a(x, y_1 + y_2) &= a(x, y_1) + a(x, y_2) \\ a(\lambda x, y) &= \lambda a(x, y) \\ a(x, \lambda y) &= \bar{\lambda} a(x, y) \end{aligned}$$

for all $x, x_1, x_2, y, y_1, y_2 \in V$ and for all $\lambda \in \mathbb{C}$. We say the form is symmetric if $a(x, y) = \overline{a(y, x)}$ for all $x, y \in V$. If in the symmetric case additionally $a(x, x) \geq 0$ for all $x \in V$ we say that a is positive. If V is even a normed space with norm $\|\cdot\|_V$ we call a sesquilinear form on V coercive, if for some $\alpha > 0$ we have $\operatorname{Re} a(x, x) \geq \alpha \|x\|_V^2$ for all $x \in V$.

Definition 2.23 (H -elliptic form). *Let V, H be Hilbert spaces with $V \hookrightarrow H$ (cf. Definition A.14) and let $a : V \times V \rightarrow \mathbb{C}$ be a continuous sesquilinear form. We say that a is H -elliptic if for some $w \in \mathbb{R}$ the form $a_w : V \times V \rightarrow \mathbb{C}$ defined by $a_w(x, y) := a(x, y) + w \langle x, y \rangle_H$ is coercive.*

The form a_w introduced in Definition 2.23 is in fact an equivalent scalar product on V , as it is shown in the next lemma, cf. [Are, p. 41].

Lemma 2.24. *Let V, H be Hilbert spaces with $V \hookrightarrow H$ and let $a : V \times V \rightarrow \mathbb{C}$ be a positive and H -elliptic form. Then a_w , as introduced in Definition 2.23, is an equivalent scalar product on V for all $w > 0$.*

Proof. Since a is a positive (and thus also a symmetric) sesquilinear form, it follows that a_w , as a sum of two scalar products on V , is a scalar product too. If we denote the norm induced by a_w as $\|x\|_w := \sqrt{a_w(x, x)}$ we have to show that there exist $m, M > 0$ such that $m\|x\|_V \leq \|x\|_w \leq M\|x\|_V$ for all $x \in V$. But this is easy to see, since the first inequality is a direct consequence from a_w being coercive, while the second inequality follows from $V \hookrightarrow H$ (which means $\|x\|_H \leq c\|x\|_V$ for some $c > 0$). \square

We are now going the first step to associate a dissipative and self-adjoint operator with a specific sesquilinear form. Instead of taking such an operator and deducing a form from it, we will approach this matter from the other side. We will consider a specific sesquilinear form, to define an associated operator, cf. [Are, Theorem 3.4.2].

Proposition 2.25. *Let V, H be Hilbert spaces such that V is dense in H and $V \hookrightarrow H$. Let $a : V \times V \rightarrow \mathbb{C}$ be a positive, continuous and H -elliptic sesquilinear form. The operator A defined below is self-adjoint and dissipative.*

$$\begin{aligned} A : H \supset \operatorname{dom}(A) &\rightarrow H \\ \operatorname{dom}(A) &:= \{x \in V : \exists y \in H \text{ with } a(x, z) = \langle y, z \rangle_H \forall z \in V\} \\ Ax &:= -y \end{aligned}$$

Proof. Consider $x, y \in \operatorname{dom}(A)$, then by the definition of A and the positivity of a we find

$$\langle Ax, y \rangle_H = -a(x, y) = -\overline{a(y, x)} = \overline{\langle Ay, x \rangle_H} = \langle x, Ay \rangle_H$$

as well as $\langle Ax, x \rangle_H = -a(x, x) \leq 0$ showing that A is symmetric and dissipative. To prove self-adjointness of A , referring to Proposition 2.21, it only remains to be shown that $(\operatorname{Id} - A)$ is surjective. Recall, that according to Lemma 2.24 setting $w = 1$

$$a_1(x, y) := a(x, y) + \langle x, y \rangle_H$$

defines a scalar product on V which is equivalent to $\langle \cdot, \cdot \rangle_V$. Now let $y \in H$, then $F(z) := \langle z, y \rangle_H$ defines a continuous linear form on V , for which by the Riesz-Frechet Theorem A.3 exists a unique

$x \in V$ such that $a_1(z, x) = \langle z, y \rangle_H$ for all $z \in V$. Rearranging leads to $a(x, z) = \langle y - x, z \rangle_H$ for all $z \in V$ and thus $Ax = x - y$, showing that $\text{Id} - T$ is surjective indeed. \square

Definition 2.26 (Associated operator). *The operator A defined in Proposition 2.25 is called the operator associated with a .*

So far we deduced an operator A associated with a given continuous, positive and H -elliptic sesquilinear form a . To justify the terminology we still have to show, that in this context the associated operator A is well defined, that is we need to show existence and uniqueness. Before we do that, we introduce the following terminology, cf. [Are, Definition 3.4.4].

Definition 2.27 (Closed positive form). *Let V, H be Hilbert spaces such V is dense in H and $V \hookrightarrow H$. Moreover let $a : V \times V \rightarrow \mathbb{C}$ be a positive, continuous and H -elliptic sesquilinear form. Then we call the pair (V, a) a closed positive form.*

To show that every dissipative self-adjoint operator A can be associated with a unique closed positive form (V, a) such that A is associated with a we have to use the spectral theorem, which is given in Theorem A.11. It states that every dissipative self-adjoint operator is unitarily equivalent to a simple multiplication operator. For the next result we refer to [Are, Theorem 3.4.5].

Proposition 2.28. *Let H be a separable Hilbert space, and let $A : H \supset \text{dom}(A) \rightarrow H$ be dissipative and self-adjoint. Then there exists a unique closed positive form (V, a) on H such that A is associated with a .*

Proof. To show uniqueness, assume (V, a) be a closed positive form, such that A is the operator associated with a . We equip V with the scalar product $a_1(x, y) := a(x, y) + \langle x, y \rangle_H$ which is equivalent to $\langle x, y \rangle_V$ as we showed in Lemma 2.24 and use this scalar product to show that $\text{dom}(A)$ is dense in V . To that end let $y \in V$ such that $a_1(x, y) = 0$ for all $x \in \text{dom}(A)$. Using Definition 2.26 it follows

$$\begin{aligned} a_1(x, y) &= \langle -Ax, y \rangle_H + \langle x, y \rangle_H \\ &= \langle (\text{Id} - A)x, y \rangle_H = 0 \quad \text{for all } x \in \text{dom}(A). \end{aligned}$$

Since A is self-adjoint and dissipative, $(\text{Id} - A)$ is surjective (see Proposition 2.21), which implies $y = 0$, and thereby density of $\text{dom}(A)$ in V . If now (W, \tilde{a}) is another closed positive form such that A is associated with \tilde{a} , then $\text{dom}(A)$ is dense in W and by Definition 2.26 it follows that both equivalent norms given by

$$\begin{aligned} \sqrt{\tilde{a}_1(x, x)} &:= \sqrt{\tilde{a}(x, x) + \langle x, x \rangle_H} = \sqrt{\|Ax\|_H^2 + \|x\|_H^2} \quad \text{for all } x \in \text{dom}(A) \\ \sqrt{a_1(x, x)} &= \sqrt{a(x, x) + \langle x, x \rangle_H} = \sqrt{\|Ax\|_H^2 + \|x\|_H^2} \quad \text{for all } x \in \text{dom}(A) \end{aligned}$$

are identical for all $x \in \text{dom}(A)$ as well as both forms $\tilde{a}(x, y) = -\langle Ax, y \rangle_H = a(x, y)$ for all $x, y \in \text{dom}(A)$. By the density of $\text{dom}(A)$ in V and the continuity of the forms a, \tilde{a} , this shows that $a = \tilde{a}$ and $W = V$, hence uniqueness of (V, a) .

For the other half of the proof, we will only give a sketch, since in order to show the existence of a closed positive form (V, a) , we have to utilize the spectral theorem, that is Theorem A.11. It allow us to assume that H is a measure space $H = L^2(\Omega, \Sigma, \mu)$ where we can express A by a multiplication operator $Af = mf$ with $\text{dom}(A) = \{f \in H : mf \in H\}$ and a measurable function $m : \Omega \rightarrow [0, \infty)$. We are now going to explicitly define a closed positive form (V, a) such that A is associated with a . To that end define V and its scalar product by

$$\begin{aligned} V &:= \{f \in L^2(\Omega, \Sigma, \mu) : \int_{\Omega} m|f|^2 d\mu < \infty\} \\ \langle f, g \rangle_V &:= \int_{\Omega} f\bar{g}(1 + m) d\mu. \end{aligned}$$

Now one can show that $(V, \langle \cdot, \cdot \rangle_V)$ is a Hilbert space that is densely embedded in H . To define the form a such that A is associated with a consider

$$a(f, g) := \int_{\Omega} f\bar{g}m d\mu$$

then (V, a) is a closed positive form such that A is associated with a . \square

Definition 2.29 (Associated form). *Let H be a separable Hilbert space, and $A : H \supset \text{dom}(A) \rightarrow H$ be dissipative and self-adjoint. The according to Proposition 2.28 well defined closed positive form (V, a) such that A is associated with a is called the form associated with A .*

So far we can only deduce self-adjointness and dissipativity of an operator A from the form (V, a) associated with it. The next result addresses a criterion how we can show that A has compact resolvent by analyzing the associated form, cf. [Are, Theorem 3.4.7].

Proposition 2.30. *Let (V, a) be a closed positive form on the Hilbert space H , and let $A : H \supset \text{dom}(A) \rightarrow H$ be the operator associated with a . If $V \xrightarrow{c} H$ then A has compact resolvent.*

Proof. According to Lemma 2.7 it suffices to show that $(\text{dom}(A), \|\cdot\|_A)$ is compactly embedded in $(H, \|\cdot\|)$. To that end, we note that $(\text{dom}(A), \|\cdot\|_A) \hookrightarrow (V, \|\cdot\|_V)$ is continuous. This follows from Lemma 2.24, since $a_1(x, x)^{1/2}$ is an equivalent norm on V . As $(V, \|\cdot\|_V) \hookrightarrow (H, \|\cdot\|)$ is compact, also $(\text{dom}(A), \|\cdot\|_A) \hookrightarrow (H, \|\cdot\|)$ is compact as the composition of a continuous and a compact embedding. \square

2.2 Combinatorial graphs and related matrices

A compilation of notions and results from the theory of finite combinatorial graphs, alongside with related theorems from linear algebra are presented below. The main sources for this section have been [KB12, Section 8.4] and [vB85].

2.2.1 Combinatorial graphs

We will use the notation $\Gamma = (V, E)$ for a given graph with the sets of vertices V and edges E both of which we assume to be nonempty, i.e., $V, E \neq \emptyset$. We will confine our considerations to finite graphs, allowing us to use the notation $V = \{v_1, \dots, v_n\}$ and $E = \{e_1, \dots, e_N\}$ with $n, N \in \mathbb{N}$ denoting the number of vertices and edges respectively. We will call two vertices $v_i, v_j \in V$ adjacent, denoted as $v_i \sim v_j$, if there exists an edge $e \in E$ with $e = \{v_i, v_j\}$. In this context the following index mapping will turn out to be convenient, cf. [vB85, p. 311].

Definition 2.31. *Let $\Gamma = (V, E)$ be a combinatorial graph with a given vertex- and edge-numbering $I_V := \{1, \dots, n\}$ and $I_E := \{1, \dots, N\}$. We define the index mapping $s : I_V \times I_V \rightarrow I_E$ as*

$$s(i, j) := \begin{cases} k & \text{if } e_k = \{v_i, v_j\} \\ 1 & \text{else.} \end{cases}$$

We will assign each edge $e = \{v_i, v_j\} \in E$ a specific direction, classifying the two adjacent vertices v_i, v_j into a start-vertex and an end-vertex. If v_i is the start- and v_j the end-vertex we will denote for the directed edge $e = (v_i, v_j)$. Additionally we will use the notation $o(e) = v_i$ and $t(e) = v_j$ to refer to the start- and end-vertex of a given directed edge $e = (v_i, v_j)$ respectively. As customary we will denote the degree of a vertex $v \in V$ with $\gamma_v := |\{e \in E : v \in e\}|$ assuming that $\gamma_v > 0$ for all $v \in V$. Moreover we will write $E_v := \{e \in E : v \in e\}$ for the set of all edges $e \in E$ that contain the vertex v . Finally all graphs considered here will be assumed to be simple and connected, i.e., containing neither multi-edges nor loops, and every two distinct vertices $v_i, v_j \in V$ can be connected by a path (cf. Definition B.10). We summarize our assumptions.

Assumption 2.32 (Combinatorial graph). *The combinatorial graph $\Gamma = (V, E)$ is assumed to be nonempty, directed, connected, finite and simple. Additional conditions might be added.*

2.2.2 Matrices associated with combinatorial graphs

The internal structure of a finite graph, regarding both the adjacency situation as well as the orientation of the edges, can be conveniently described by the means of matrices. In this section we will present the matrices we need to do so. We will encounter the so called adjacency matrix \mathcal{A} , the transition matrix \mathcal{Z} , and the signed incidence matrix \mathcal{D} .

We begin with the adjacency matrix. As the name suggests this matrix summarizes the adjacency structure of our graph, cf. [KB12, Definition 8.39].

Definition 2.33 (Adjacency matrix). Let $\Gamma = (V, E)$ be a graph satisfying Assumption 2.32 with vertices $V = \{v_1, v_2, \dots, v_n\}$. We define the adjacency matrix $\mathcal{A}(\Gamma) := (e_{ij}) \in \{0, 1\}^{n \times n}$ by

$$e_{ij} = \begin{cases} 1 & \text{if } v_i \sim v_j \\ 0 & \text{if } v_i \not\sim v_j. \end{cases}$$

Most of the time we will just write \mathcal{A} instead of $\mathcal{A}(\Gamma)$. Also we will sometimes write $e_{v,w}$ with vertices $v, w \in V$ for an element in \mathcal{A} when we did not introduce a numbering of the vertices. The next proposition shows two basic properties of the adjacency matrix \mathcal{A} when we are considering connected graphs, as we assumed it in Assumption 2.32, see [KB12, 8.42, 8.43].

Proposition 2.34. *The adjacency matrix $\mathcal{A}(\Gamma)$ of a connected combinatorial graph $\Gamma = (V, E)$ satisfying Assumption 2.32 is symmetric and irreducible.*

Proof. The symmetry of \mathcal{A} is a direct consequence from the adjacency relation \sim being symmetric, that is $v_i \sim v_j$ if and only if $v_j \sim v_i$. For the second part of the assertion assume that \mathcal{A} is reducible (see Definition B.2), that is, there exists a permutation matrix $P \in \mathbb{R}^{n \times n}$ such that

$$P\mathcal{A}P^T = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}.$$

with $A_{11} \in \mathbb{R}^{r \times r}$ and $A_{22} \in \mathbb{R}^{(n-r) \times (n-r)}$ for some $\mathbb{N} \ni r < n$ where $n = |V|$. Here we used the symmetry of \mathcal{A} . But this implies that we can find disjoint $V_1, V_2 \subset V$ with $V_1 \cup V_2 = V$ such that $v_1 \not\sim v_2$ for all $v_1 \in V_1$ and $v_2 \in V_2$, that is Γ is not connected. This shows that \mathcal{A} is irreducible. \square

The adjacency matrix will play an important role in the so called adjacency calculus discussed in Section 3.2.2. In the same context we will also encounter the so called transition matrix \mathcal{Z} , which is derived from the adjacency matrix, and plays an important role in our quantitative analyses in Section 3.2.2, cf. [vB85, p. 317].

Definition 2.35 (Transition matrix). Let Γ be a combinatorial graph satisfying Assumption 2.32 with adjacency matrix \mathcal{A} . Using $e := (1)_{n \times 1}$, we define the transition matrix $\mathcal{Z} \in \{0, 1\}^{n \times n}$ as

$$\mathcal{Z}(\Gamma) := \text{Diag}(\mathcal{A}e)^{-1}\mathcal{A}.$$

Here, as customary, the Diag operator maps a vector $v = (v_i) \in \mathbb{C}^n$ to a corresponding diagonal matrix $V = (v_{ij}) \in \mathbb{C}^{n \times n}$ with $v_{ii} = v_i$ for all $i \in \{1, \dots, n\}$.

We will now take a closer look on the properties of the transition matrix. As it has been said before, we are mostly interested in information on the eigenvalues, cf. [vB85, p. 317] and [vB84].

Lemma 2.36. *Let Γ be a graph satisfying Assumption 2.32 with adjacency matrix \mathcal{A} . Then the transition matrix \mathcal{Z} is irreducible and row-stochastic. Moreover \mathcal{Z} has only real eigenvalues $\mu_1, \dots, \mu_n \in \mathbb{R}$ which can be sorted, taking into account their multiplicities, as*

$$1 = \mu_1 > \mu_2 \geq \dots \geq \mu_n \geq -1. \quad (1)$$

Furthermore, if $\mu_n = -1$ then Γ is bipartite.

Proof. From Proposition 2.34 we know that \mathcal{A} is irreducible, which by the Definition 2.35 of \mathcal{Z} shows that \mathcal{Z} is irreducible as well. Since \mathcal{Z} is derived from the adjacency matrix by dividing each row by its row-sum, \mathcal{Z} is obviously row-stochastic.

We will now show that all eigenvalues are indeed real. To that end we define the positive definite matrix $D := \text{Diag}(\mathcal{A}e)$ and the symmetric matrix $W := D^{-1/2}\mathcal{A}D^{-1/2}$ where the exponent $-1/2$ applies on each diagonal element of D . Let now $v \in \mathbb{C}^n$ be an eigenvector of \mathcal{Z} corresponding to the eigenvalue μ , then we obtain with $\tilde{v} := D^{1/2}v$ (again the exponent just applies on the diagonal)

$$\begin{aligned} \mathcal{Z}v = \mu v &\Leftrightarrow \mathcal{A}v = \mu Dv \\ &\Leftrightarrow \mathcal{A}D^{-1/2}D^{1/2}v = \mu D^{1/2}D^{1/2}v \\ &\Leftrightarrow D^{-1/2}\mathcal{A}D^{-1/2}\tilde{v} = \mu\tilde{v} \\ &\Leftrightarrow W\tilde{v} = \mu\tilde{v} \end{aligned}$$

hence $\sigma(\mathcal{Z}) = \sigma(W)$. With the symmetry of W this shows that $\sigma(\mathcal{Z})$ is real. Now using Proposition B.4 we conclude that $\sigma(\mathcal{Z}) \in [-1, 1]$. Additionally we know from the theorem of Perron-Frobenius B.5 that the eigenvalue $\lambda = 1$ is simple, which in summary shows that (1) holds.

This brings us to the last part of the assertion. Assume that $\mu_n = -1$ is an eigenvalue of \mathcal{Z} , then -1 is also an eigenvalue of the symmetric matrix W corresponding to some eigenvector $0 \neq \tilde{w} = D^{1/2}w$ with $\mathcal{Z}w = -w$. Since also $1 \in \sigma(\mathcal{Z})$ we know that 1 is an eigenvalue of W too, corresponding to a strictly positive eigenvector $\tilde{u} = D^{1/2}u > 0$ by the theorem of Perron-Frobenius. Note that in this context $\mathcal{Z}u = u$ and hence $u = e$. Now, due to $|\tilde{w}| = |-\tilde{w}| = |W\tilde{w}| \leq W|\tilde{w}|$ (because W only contains positive entries) we find

$$\tilde{u}^T |\tilde{w}| \leq \tilde{u}^T W |\tilde{w}| = (W\tilde{u})^T |\tilde{w}| = \tilde{u}^T |\tilde{w}|$$

which implies that $W|\tilde{w}| = |\tilde{w}|$. We conclude that \tilde{w} has no zero elements since $|\tilde{w}|$ is an eigenvector corresponding to $\mu_1 = 1$ and by the theorem of Perron-Frobenius, which states $|\tilde{w}| > 0$. Due to $|\tilde{w}| = c\tilde{u}$ for some $c > 0$ and $\tilde{w} \neq \tilde{u} > 0$ (both correspond to different eigenvalues) we can assume \tilde{w} to have positive and negative elements. If we now recall from before that $\tilde{u} := D^{1/2}e$ with $e = (1)_{n \times 1}$ and $\tilde{w} := D^{1/2}w$ we conclude that an eigenvector $w = (w_i)$ of \mathcal{Z} corresponding to the eigenvalue $\mu_n = -1$ only contains ± 1 elements due to $|w| = ce$ with $c > 0$. If we sort the indices of the w_i in the subsets P and N , that is $w_i > 0$ for all $i \in P$ and $w_i < 0$ for all $i \in N$ we obtain by considering $\mathcal{Z}w = -w$ and setting $\mathcal{Z} = (z_{ij})$ that

$$\begin{aligned} \sum_{j \in P} z_{ij} - \sum_{j \in N} z_{ij} &= 1 \quad \text{for all } i \in N \\ \sum_{j \in P} z_{ij} - \sum_{j \in N} z_{ij} &= -1 \quad \text{for all } i \in P. \end{aligned}$$

This implies, since $\mathcal{Z} = (z_{ij})$ is row-stochastic, that $z_{ij} = e_{ij} = 0$ for all $(i, j) \in N \times N$ on the one hand and $z_{ij} = e_{ij} = 0$ for all $(i, j) \in P \times P$ on the other. Hence in P and N we found a bipartition of V showing that Γ is bipartite. \square

So far we know, that whenever we find $\mu_n = 1$ in the spectrum of $\mathcal{Z}(\Gamma)$ that Γ is bipartite. In the next lemma we will see, that the converse also holds. In fact, we can even show more.

Lemma 2.37. *Let Γ be a connected graph. The eigenvalues of $\mathcal{Z}(\Gamma)$ are symmetric with respect to 0 if and only if Γ is bipartite.*

Proof. At first assume that $\Gamma = (V, E)$ is bipartite, hence we can find two disjoint subsets $A, B \subset V$ with $A \cup B = V$ such that each of the subsets A, B is not interconnected, that is for each $e \in E$ we have $e \cap A \neq \emptyset$ and $e \cap B \neq \emptyset$. If we now label the vertices by first numbering all vertices from A and then all vertices from B , that is

$$V = \underbrace{\{v_1, v_2, \dots, v_{n_A}\}}_A \underbrace{\{v_{n_A+1}, v_{n_A+2}, \dots, v_{n_A+n_B}\}}_B \quad (2)$$

we see that the adjacency matrix \mathcal{A} corresponding to these vertex labels is of the form

$$\mathcal{A} = \begin{pmatrix} 0 & M \\ M^T & 0 \end{pmatrix}$$

where M is a $n_A \times n_B$ -matrix. Taking into account the definition of \mathcal{Z} we find the structure

$$\mathcal{Z} = \begin{pmatrix} 0 & M_A \\ M_B & 0 \end{pmatrix}$$

with the $n_A \times n_B$ -matrices M_A and M_B . Now assume that $\lambda \neq 0$ is an eigenvalue of \mathcal{Z} corresponding to the eigenvector $v = (v_A, v_B)^T$ which we split in the same way as indicated in (2). We compute

$$\mathcal{Z}v = \begin{pmatrix} 0 & M_A \\ M_B & 0 \end{pmatrix} \begin{pmatrix} v_A \\ v_B \end{pmatrix} = \begin{pmatrix} M_A v_B \\ M_B v_A \end{pmatrix} = \begin{pmatrix} \lambda v_A \\ \lambda v_B \end{pmatrix} = \lambda v.$$

If we now consider the vector $v' := (-v_A, v_B)^T$ we obtain

$$\mathcal{Z}v' = \begin{pmatrix} 0 & M_A \\ M_B & 0 \end{pmatrix} \begin{pmatrix} -v_A \\ v_B \end{pmatrix} = \begin{pmatrix} M_A v_B \\ -M_B v_A \end{pmatrix} = \begin{pmatrix} \lambda v_A \\ -\lambda v_B \end{pmatrix} = -\lambda \begin{pmatrix} -v_A \\ v_B \end{pmatrix} = -\lambda v'$$

from which we see that $-\lambda$ is an eigenvalue of \mathcal{Z} too. The converse implication is a direct consequence from Lemma 2.36 since the symmetry of the eigenvalues especially results in $\lambda = -1$ being an eigenvalue of \mathcal{Z} . Combining both results we arrive at the assertion. \square

The combinatorial graphs that we consider here mostly contain two structures - the adjacency structure describing which vertices are adjacent, and the direction structure describing the directions assigned to the edges of the graph. So far we only considered the adjacency structure - now we turn to the structure of directions, which is described by the so-called signed incidence matrix, cf. [vB85, p. 311].

Definition 2.38 (Signed incidence matrix). *Let $\Gamma = (V, E)$ be a graph satisfying Assumption 2.32, with vertices $V = \{v_1, v_2, \dots, v_n\}$ and edges $E = \{e_1, e_2, \dots, e_N\}$. We define the signed incidence matrix $\mathcal{D}(\Gamma) := (d_{ij}) \in \{-1, 0, 1\}^{n \times N}$ by*

$$d_{ij} = \begin{cases} -1 & \text{if } v_i = o(e_j) \\ 1 & \text{if } v_i = t(e_j) \\ 0 & \text{else.} \end{cases}$$

The last case in the definition above obviously holds when the vertex v_i is not contained in the edge e_j . Most of the times we will just write \mathcal{D} instead of $\mathcal{D}(\Gamma)$. Also we will sometimes write $d_{v,e}$ with a vertex $v \in V$ and an edge $e \in E$ for an element in \mathcal{D} when we did not introduce a numbering of the vertices and edges. The following two results provide us with information on the rank of \mathcal{D} and its kernel, see [Jun08, Theorem 4.2.4].

Lemma 2.39 (Rank of \mathcal{D}). *Let $\Gamma = (V, E)$ be a graph satisfying Assumption 2.32 with n vertices and the signed incidence matrix \mathcal{D} . Then $\text{rank}(\mathcal{D}) = n - 1$.*

Proof. At first we note that each column of \mathcal{D} contains exactly one $+1$ and one -1 entry, while the remaining values are zero. Summing up all n row vectors $r_i := (d_{i,1}, \dots, d_{i,N})$ we hence obtain the zero-vector showing that $\text{rank}(\mathcal{D}) < n$. Now assume $\sum c_i r_i = 0$ would be another row vector sum resulting in the zero vector with at least one $c_k \neq 0$. Using again the property that each column is filled with zeros except from exactly one ± 1 pair, next to Γ being connected, we conclude that $c_i = c_k \neq 0$ for all $i \in \{1, \dots, n\}$. Since this is the case we started with we see that $\text{rank}(\mathcal{D}) = n - 1$, which is the assertion. \square

Corollary 2.40. *Let $\Gamma = (V, E)$ be a graph satisfying Assumption 2.32 with n vertices, N edges and the signed incidence matrix \mathcal{D} . Then $\dim(\ker(\mathcal{D})) = N - n + 1$.*

Proof. Since \mathcal{D} maps into an N -dimensional space we have $N = \dim(\ker(\mathcal{D})) + \text{rank}(\mathcal{D})$ which immediately gives $\dim(\ker(\mathcal{D})) = N - n + 1$ by using Lemma 2.39. \square

2.3 The notion of a quantum graph

In this section the notion of a quantum graph will be introduced. A quantum graph is a pair (Γ_l, \mathcal{H}) consisting of a metric graph Γ_l and a specific differential operator \mathcal{H} , often referred to as the Hamiltonian of the quantum graph. Both of these objects relate to each other as the metric graph is used to define the domain of the Hamiltonian. One usually expresses this situation by saying that \mathcal{H} is acting on Γ_l or that Γ_l is equipped with \mathcal{H} .

In the following we will develop the notions of both the metric graph and the Hamiltonian, where we follow the introduction given by Berkolaiko and Kuchment in [BK13, Section 1.1-1-4].

2.3.1 Metric graphs

A metric graph is a combinatorial graph whose edges have been assigned specific lengths or weights. This allows us to define a metric on this type of graph, which justifies the term *metric* graph. A formal definition is given below, cf. [Kuc04, Definition 1]

Definition 2.41 (Metric graph). *A metric graph $\Gamma_l := (\Gamma, l)$ is a pair consisting of a combinatorial graph $\Gamma = (V, E)$ and a function $l : E \rightarrow (0, \infty]$ with $e \mapsto l(e) =: l_e$. If $|V| < \infty$ and $l_e < \infty$ for all $e \in E$ we say that Γ_l is compact. If even $l_e = 1$ for all $e \in E$ the metric graph is called equilateral.*

It is easy to see, that we can define a simple path metric (cf. Definition B.10) on compact metric graphs by defining the distance between two vertices as the shortest weighted path connecting them, see [Mug17, Example 1.1.3].

Proposition 2.42 (Graph metric). *Let $\Gamma_l = (\Gamma, l)$ be a compact metric graph, with Γ in line with Assumption 2.32. Then we can define a metric $d : V \times V \rightarrow [0, \infty)$ by setting*

$$d(u, v) := \min \left\{ \sum_{e \in p} l_e : p \text{ is a path from } u \text{ to } v \right\}.$$

We forgo the elementary proof. A compact metric graph with an underlying directed combinatorial graph according to Assumption 2.32 allows us to interpret an edge $e \in E$ of such a graph as a one dimensional real interval $[0, l_e]$ with the origin in $o(e)$ and the end in $t(e)$, that is with a direction inherited from the directional structure of Γ .

If we identify each edge of Γ_l with an interval we can define functions on the edges of the graph, and thereby on the graph in total [BK13, Definition 1.3.7].

Definition 2.43 (Graph function spaces). *Let $\Gamma_l = (\Gamma, l)$ be a compact metric graph with $\Gamma = (V, E)$ in line with Assumption 2.32, and where each edge $e \in E$ is identified with the interval $[0, l_e]$ as described before. With $1 \leq p < \infty$ and $k \in \mathbb{N}_0$ we set $L^p(e) := L^p(0, l_e)$ and $H^k(e) := H^k(0, l_e)$. Moreover we define the graph function spaces $(\tilde{L}^p(\Gamma), \|\cdot\|_{\tilde{L}^p})$ and $(\tilde{H}^k(\Gamma), \|\cdot\|_{\tilde{H}^k})$ by*

$$\begin{aligned} \tilde{L}^p(\Gamma) &:= \bigoplus_{e \in E} L^p(e) \quad \text{with} \quad \|f\|_{\tilde{L}^p(\Gamma)}^2 := \sum_{e \in E} \|f\|_{L^p(e)}^2, \quad f \in \tilde{L}^p(\Gamma) \\ \tilde{H}^k(\Gamma) &:= \bigoplus_{e \in E} H^k(e) \quad \text{with} \quad \|f\|_{\tilde{H}^k(\Gamma)}^2 := \sum_{e \in E} \|f\|_{H^k(e)}^2, \quad f \in \tilde{H}^k(\Gamma). \end{aligned}$$

One can easily check that $\tilde{L}^2(\Gamma)$ and $\tilde{H}^k(\Gamma), k \in \mathbb{N}$ are in fact Hilbert spaces with respect to the scalar product $\langle f, g \rangle_{\tilde{L}^2(\Gamma)} := \sum_{e \in E} \langle f, g \rangle_{L^2(e)}$ and $\langle f, g \rangle_{\tilde{H}^k(\Gamma)} := \sum_{e \in E} \langle f, g \rangle_{H^k(e)}$ respectively.

This already concludes our review on metric graphs. For easier reference we will summarize our most frequently assumed properties of the metric graphs in the following

Assumption 2.44 (Metric graph). *The metric graph $\Gamma_l = (\Gamma, l)$ with $\Gamma = (V, E)$ according to Assumption 2.32 is assumed to be compact and equilateral. Moreover we associate Γ_l with the graph function spaces $(\tilde{L}^p(\Gamma), \|\cdot\|_{\tilde{L}^p})$ and $(\tilde{H}^k(\Gamma), \|\cdot\|_{\tilde{H}^k})$ introduced in Definition 2.43.*

2.3.2 The Hamiltonian

The so-called Hamiltonian \mathcal{H} is the differential operator of a quantum graph (Γ_l, \mathcal{H}) . The definition of the Hamiltonian incorporates a metric graph Γ_l , a set of classical differential operators, each of which is assigned to an edge of the graph (or, to be more precise, to the function spaces associated with the edges of Γ_l) and finally a set of so-called vertex conditions, which state conditions for graph functions to be in $\text{dom}(\mathcal{H})$ referring to their values and derivatives at the vertices of Γ_l .

Considering the classical differential operators which are assigned to the function spaces associated with the edges of Γ_l , we note that in applications these operators are usually defined in a similar fashion. This allows one to just define one classical differential operator, which is then applied on each edge separately. Referring to [BK13, p. 12] the most common operators are

(Negative) Standard Laplacian	$f_e \mapsto -\frac{d^2}{dx_e^2} f_e$
General Schrödinger operator	$f_e \mapsto \left(-\frac{d^2}{dx_e^2} + V(x_e) \right) f(x_e)$
Magnetic Schrödinger operator	$f_e \mapsto \left(\frac{1}{i} \frac{df_e}{dx_e} - A(x_e) \right)^2 f(x_e) + V(x_e) f(x_e)$

where x_e refers to the coordinate associated with the interval $[0, l_e]$ associated with the edge $e \in E$, and V, A are potential function defined on a space the graph is embedded in.

For the remainder of this subsection, as for the remainder of the thesis, we are going to focus on quantum graphs constituted by a compact metric graph in line with Assumption 2.44 (we will call such quantum graphs consequently *compact* quantum graphs), and the standard Laplacian as introduced above. The latter we will usually denote as $-\Delta$.

To completely define $-\Delta$ on Γ_l we have to describe its domain. So far, by the definition of the metric graph Γ_l summarized in Assumption 2.44, we just implied that $f \in \text{dom}(\mathcal{H})$ whenever $f \in \tilde{L}^p(\Gamma)$ or $f \in \tilde{H}^k(\Gamma)$, depending on the considered graph function space. But which function space should we use in this case specifically? It is clear, that we cannot use $\tilde{L}^p(\Gamma)$ as the domain for $-\Delta$, since not all functions in $L^p(e), e \in E$ are differentiable. To overcome this problem one might think to simply use $\tilde{C}^2(\Gamma)$ instead of $\tilde{L}^p(\Gamma)$, where its definition would be analogous to Definition 2.43. However, $\tilde{C}^2(\Gamma)$ is neither closed nor dense in $\tilde{L}^p(\Gamma)$. To account for density we could switch to $\tilde{C}_0^\infty(\Gamma)$, but the problem remains that also $\tilde{C}_0^\infty(\Gamma)$ is not closed in $\tilde{L}^2(\Gamma)$ and would result in $\sigma(\mathcal{H}) = \mathbb{C}$. Only its closure in $\tilde{L}^2(\Gamma)$, that is $\tilde{H}_0^2(\Gamma)$, finally gives us a reasonable (because closed) domain for our Hamiltonian. We will hence use $\text{dom}(-\Delta) = \tilde{H}_0^2(\Gamma)$ for our next considerations.

Although we now have a Hamiltonian with closed domain, it does not make a lot of sense yet if we want to capture the nature of the underlying graph structure. The reason for that is that the edge functions are pairwise independent - they do not communicate with each other. If we change a single edge-function, we do not have to change any other function in response. However, as soon as we introduce vertex conditions the situation changes. Considering any vertex $v \in V$, the vertex conditions state requirements for f to be in the domain of \mathcal{H} with respect to the values and derivatives of all edge-functions f_e defined on edges that share the vertex v . Two examples for such vertex conditions, which are also the conditions considered in this thesis, are the so-called Kirchhoff and Anti-Kirchhoff vertex conditions. Referring to [vBM13, Section 3] they are defined by requiring for each $v \in V$ that

$$\text{Kirchhoff conditions (CK)} : \begin{cases} f_e(v) = f_{\bar{e}}(v) \quad \forall e, \bar{e} \in E_v \\ \sum_{e \in E_v} d_{v,e} f'_e(v) = 0. \end{cases}$$

$$\text{Anti-Kirchhoff conditions (KC)} : \begin{cases} d_{e,v} f'_e(v) = d_{\bar{e},v} f'_{\bar{e}}(v) \quad \forall e, \bar{e} \in E_v \\ \sum_{e \in E_v} d_{v,e}^2 f_e(v) = 0. \end{cases}$$

where $d_{v,e}$ refers to the values of the signed incidence matrix \mathcal{D} , cf. Definition 2.38, and E_v denotes the set of all edges that contain v , cf. Section 2.2.

Note that the values $f_e(v_i)$ and derivatives $f'_e(v_i)$ of the edge function at the vertices $v_i \in V$ are well defined whenever $f_e \in H^2(e)$ due to Theorem A.13.

Looking back at the vertex conditions, we notice that every $f \in \tilde{H}_0^2(\Gamma)$ satisfies both Kirchhoff and Anti-Kirchhoff conditions. From that perspective one can understand the requirement of these vertex conditions as the extension of $\text{dom}(-\Delta) = \tilde{H}_0^2(\Gamma)$ to $\{f \in \tilde{H}^2(\Gamma) : f \text{ satisfies CK}\} \supset \tilde{H}_0^2(\Gamma)$ and $\{f \in \tilde{H}^2(\Gamma) : f \text{ satisfies KC}\} \supset \tilde{H}_0^2(\Gamma)$ respectively. Since the standard Laplacian on these domains are the central objects in this thesis, we summarize their definition.

Definition 2.45 (Considered Hamiltonians). *Let $\Gamma_l = (\Gamma, l)$ be a metric graph in line with Assumption 2.44, and set $\tilde{H}_{CK}^2 := \{f \in \tilde{H}^2(\Gamma) : f \text{ satisfies CK}\}$ and $\tilde{H}_{KC}^2 := \{f \in \tilde{H}^2(\Gamma) : f \text{ satisfies KC}\}$. We define the Hamiltonians $-\Delta_\Gamma^{CK}$ and $-\Delta_\Gamma^{KC}$ by*

$$\begin{aligned} -\Delta_\Gamma^{CK} : \tilde{L}^2(\Gamma) \supset \tilde{H}_{CK}^2(\Gamma) &\rightarrow \tilde{L}^2(\Gamma) \quad \text{with} \quad f_e \mapsto -\frac{d^2 f_e}{dx_e^2} \quad \forall e \in E \\ -\Delta_\Gamma^{KC} : \tilde{L}^2(\Gamma) \supset \tilde{H}_{KC}^2(\Gamma) &\rightarrow \tilde{L}^2(\Gamma) \quad \text{with} \quad f_e \mapsto -\frac{d^2 f_e}{dx_e^2} \quad \forall e \in E. \end{aligned}$$

3 Spectral analyses

This section contains the spectral analyses of the standard Laplacian on bounded one dimensional intervals (Section 3.1) and on finite equilateral metric graphs (Section 3.2). For both domains two kinds of boundary/vertex conditions are considered. In the first case we consider Dirichlet and Neumann conditions, while in the second case we distinguish between Kirchhoff and Anti-Kirchhoff conditions. Note that the first analysis can be interpreted as a special case of the second analysis by considering a bounded interval as a graph with one edge and two vertices. Moreover, the Dirichlet and Neumann boundary conditions can be understood as Anti-Kirchhoff and Kirchhoff vertex conditions respectively.

Each analysis is subdivided into three parts, that is a qualitative spectral analysis, a quantitative spectral analysis and finally a comparison of the spectra with respect to the distinguished boundary/vertex conditions. While the qualitative analysis focuses on general properties of the spectra, we actually compute the spectra in the quantitative analysis. Finally, we compare the results for both boundary/vertex conditions and analyze how the spectra might be related.

3.1 The standard Laplacian on bounded intervals

In the following we will analyze the spectrum of the standard Laplacian $-\Delta$ on a bounded one dimensional interval under Dirichlet and Neumann boundary conditions respectively. For most of these results we refer to [Are, Section 3] and to our results from Section 2.1.3.

To provide a general reference and fully formulate the spectral problem we are considering in this subsection, we state the following

Problem 3.1. *Let $a, b \in \mathbb{R}$ such that $a < b$. Consider the two Laplacians*

$$\text{Dirichlet Laplacian} := \begin{cases} -\Delta^D & : L^2(a, b) \supset \text{dom}(-\Delta^D) \rightarrow L^2(a, b) \\ \text{dom}(-\Delta^D) & := \{f \in H^2(a, b) : f(a) = f(b) = 0\} \\ -\Delta^D f & := -f'' \end{cases}$$

$$\text{Neumann Laplacian} := \begin{cases} -\Delta^N & : L^2(a, b) \supset \text{dom}(-\Delta^N) \rightarrow L^2(a, b) \\ \text{dom}(-\Delta^N) & := \{f \in H^2(a, b) : f'(a) = f'(b) = 0\} \\ -\Delta^N f & := -f''. \end{cases}$$

Find $\lambda_D \in \mathbb{C}$ and $0 \neq u \in \text{dom}(-\Delta^D)$, as well as $\lambda_N \in \mathbb{C}$ and $0 \neq v \in \text{dom}(-\Delta^N)$ such that

$$-\Delta^D u = \lambda_D u$$

$$-\Delta^N v = \lambda_N v.$$

3.1.1 Qualitative analysis

To qualitatively analyze the operators presented in Problem 3.1, we use two different approaches, both of which are outlined in [Are, Section 3]. At first we are going to consider the Dirichlet Laplacian. We will show that this operator is nonnegative, self-adjoint and has compact resolvent. The central means to show that will be the representation theorem of Riesz-Fréchet (see Theorem A.3) in combination with the range condition as criterion for self-adjointness of an operator.

For the second considered operator, the Neumann Laplacian, we will utilize the approach of associated forms, presented in Subsection 2.1.3. We will end up with the same result, as we will arrive at for the Dirichlet Laplacian, that is $-\Delta^N$ being nonnegative, self-adjoint and having compact resolvent.

Before we get to our first analysis, we note the following important result, which is an easy corollary of the Rellich-Kondrachov Theorem A.15.

Corollary 3.2. *Let $[a, b] \subset \mathbb{R}$ be a bounded real interval. Then $H^2(a, b) \xrightarrow{c} L^2(a, b)$.*

Proof. The assertion is an immediate consequence from the Rellich-Kondrachov Theorem A.15 when setting $j = 0$ and $m = p = q = 2$, since $W^{0,2}(a, b) = L^2(a, b)$. \square

The following result considers the properties of the Dirichlet Laplacian. It was derived from [Are, Theorem 3.2.1].

Proposition 3.3 (Dirichlet Laplacian). *The Dirichlet Laplacian $-\Delta^D$ defined in Problem 3.1 is nonnegative, self-adjoint and has compact resolvent.*

Proof. At first note that $\sigma(-\Delta^D) = -\sigma(\Delta^D)$. Indeed, if $\lambda \in \mathbb{C}$ and some $f \in \text{dom}(T)$ satisfies $-\Delta^D f = \lambda f$ then obviously $\Delta^D f = (-\lambda)f$. This allows us to analyze Δ^D with the domain $\text{dom}(\Delta^D) := \text{dom}(-\Delta^D)$ instead of $-\Delta^D$.

We begin by analyzing some simple properties of Δ^D . First, consider $f, g \in \text{dom}(T)$, then by partial integration, and the boundary conditions, we find

$$\langle \Delta^D f, g \rangle_{L^2(a,b)} = - \int_a^b f' \bar{g} dx = \langle f, \Delta^D g \rangle_{L^2(a,b)}$$

which shows that Δ^D is symmetric. Moreover from $\langle \Delta^D f, f \rangle_{L^2(a,b)} = - \int_a^b |f'|^2 dx \leq 0$ we see that Δ^D is also dissipative. If we now have a look at Proposition 2.21 we see that two of the three conditions that identify an operator as dissipative and self-adjoint are satisfied. It only remains to be shown that $\text{Id} - \Delta^D$ is surjective, that is $\text{ran}(\text{Id} - \Delta^D) = L^2(a, b)$.

To that end, let $g \in L^2(a, b)$, and define the continuous linear form $\Phi(\varphi) := \int_a^b \varphi \bar{g} dx$ on $H_0^1(a, b)$. By the Riesz-Fréchet Theorem A.3 there exists a unique $f \in H_0^1(a, b)$ such that for all $\varphi \in H_0^1(a, b)$

$$\Phi(\varphi) = \int_a^b \varphi \bar{g} dx = \langle \varphi, f \rangle_{H^1(a,b)} = \int_a^b \varphi \bar{f}' dx + \int_a^b \varphi' \bar{f} dx \quad (3)$$

holds. Considering $\bar{\varphi}$ instead of φ , and taking the complex conjugate of (3) leads to

$$- \int_a^b \varphi' f' dx = \int_a^b \varphi (f - g) dx$$

for all $\varphi \in C_0^\infty(a, b) \subset H_0^1(a, b)$, implying that $f - g$ is the weak derivative of f' . It follows $f \in H^2(a, b)$ with $f'' = f - g$, and therefore $f \in \text{dom}(A)$ and $(\text{Id} - \Delta^D)f = g$. This shows that Δ^D is surjective, and according to Proposition 2.21 implies that Δ^D is self-adjoint.

To show that Δ^D also has compact resolvent, we consider $(\lambda - \Delta^D)^{-1}$ for some $\lambda \in \rho(\Delta^D) \neq \emptyset$. First, note that $(\lambda - \Delta^D)^{-1}$ maps $L^2(a, b)$ continuously into $H^2(a, b) \supset \text{dom}(\Delta^D)$. Moreover, referring to Corollary 3.2, we recall that $H^2(a, b)$ is compactly embedded in $L^2(a, b)$. As a composition of a continuous and a compact operator, we see that $(\lambda - \Delta^D)^{-1} : L^2(a, b) \rightarrow L^2(a, b)$ is compact as well. This shows that Δ^D has compact resolvent.

Summarizing our results, we see that Δ^D is dissipative, self-adjoint and has compact resolvent. With the considerations from the beginning of this proof, we hence see, that $-\Delta^D$ is nonnegative, self-adjoint and has compact resolvent. \square

We continue our qualitative considerations with the Neumann Laplacian Δ^N . This time we choose a different approach using the symmetric form associated with Δ^N as we presented it in Subsection 2.1.3. We refer to [Are, Theorem 3.4.8].

Proposition 3.4 (Neumann Laplacian). *The Neumann Laplacian $-\Delta^N$ defined in Problem 3.1 is nonnegative, self-adjoint and has compact resolvent.*

Proof. With the same arguments as in Proposition 3.3, we will consider Δ^N instead of $-\Delta^N$. We are choosing this approach since Δ^N will turn out to be a dissipative operator, and is thus in line with the operators we considered in Subsection 2.1.3, when we looked at symmetric forms associated with operators.

Our strategy is to find the form associated with Δ^N (cf. Definition 2.29), show that this form is positive, continuous and H -elliptic and finally use Proposition 2.25 and 2.30 to confirm the claimed properties of Δ^N .

Considering the definition of the associated operator of a positive, continuous and H -elliptic form, as it is introduced in Proposition 2.25 we will try to reformulate $\langle -\Delta^N f, g \rangle_{L^2(a,b)}$ with

$f, g \in \text{dom}(\Delta^N)$ such that it can be interpreted as a form on a subspace of $L^2(a, b)$. Using partial integration and the boundary conditions we find

$$\langle -\Delta^N f, g \rangle = - \int_a^b f'' \bar{g} dx = \int_a^b f' \bar{g}' dx$$

which suggests to define the form $a(f, g) := \int_a^b f' \bar{g}' dx$ on $V := H^1(a, b)$. We check the properties of a . Since for all $f, g \in V$ we have

$$\begin{aligned} a(f, g) &= \int_a^b \bar{g}' f' dx = \overline{\int_a^b g' \bar{f}' dx} = \overline{a(g, f)} \\ a(f, f) &= \int_a^b f' \bar{f}' dx = \int_a^b |f'|^2 dx \geq 0 \\ |a(f, g)| &= \left| \int_a^b f' \bar{g}' dx \right| \leq M_f M_{\bar{g}} \|f'\|_V \|\bar{g}'\|_V \end{aligned}$$

with $M_f M_{\bar{g}} > 0$, where we used in the estimate of $|a(f, g)|$ that $f', \bar{g}' \in C(a, b)$. Hence a is positive and continuous. To show that a is also $L^2(a, b)$ -elliptic we simply consider

$$\begin{aligned} \|f\|_{H^1(a, b)}^2 &= \|f\|_{L^2(a, b)}^2 + \|f'\|_{L^2(a, b)}^2 \\ &= \langle f, f \rangle_{L^2(a, b)} + a(f, f). \end{aligned}$$

We hence identified a as a positive, continuous and $L^2(a, b)$ -elliptic form.

If we knew that a is actually the form associated with Δ^N we would be done at this point. But in fact we do not know that yet - a is just a promising candidate. The rest of the proof is therefore concerned with showing that the operator associated with a is identical with Δ^N .

Let A be the operator associated with our form a . Now consider $f \in \text{dom}(\Delta^N)$ with $\Delta^N f =: g$. We obtain for $h \in V$

$$\langle -g, h \rangle_{L^2(a, b)} = \langle -\Delta^N f, h \rangle_{L^2(a, b)} = \int_0^1 g' \bar{h}' dx = a(g, h).$$

Thus, by Definition 2.29 we have $f \in \text{dom}(A)$ and $Af = g$ which shows $-\Delta^N \subset A$.

For the converse inclusion assume $f \in \text{dom}(A)$ with $Af =: g$. Using the definition given in Proposition 2.25 we find for $h \in V$

$$a(f, h) = \langle -g, h \rangle_{L^2(a, b)} = - \int_a^b g \bar{h} dx = \int_a^b f' \bar{h}' dx. \quad (4)$$

Since $C_0^\infty(a, b) \subset V$ this holds especially for all $h \in C_0^\infty(a, b)$, showing that $f' \in H^1(a, b)$, thus $f \in H^2(a, b)$, which allows us to consider f'' . Partial integration in (4) gives us

$$a(f, h) = \int_a^b f' \bar{h}' dx = - \int_a^b f'' \bar{h} dx = -[f' \bar{h}]_a^b + \int_a^b f' \bar{h}' dx$$

for all $h \in V$. This shows $f'(a) = f'(b) = 0$ as well as $f'' = g$, and thereby $f \in \text{dom}(A)$. Combining both results we end up with $A = \Delta^N$, showing that Δ^N is indeed the operator associated with a . Applying Proposition 2.25 we hence conclude that Δ^N is dissipative and self-adjoint.

Finally we want to address the property of Δ^N having compact resolvent, as claimed in the assertion. According to Proposition 2.30 we can show that by checking if V is compactly embedded in $L^2(a, b)$. But this follows immediately from Corollary 3.2. We hence see, that Δ^N has compact resolvent indeed.

Applying these results on $-\Delta^N$, recalling the considerations at the beginning of Proposition 3.3, we conclude that $-\Delta^N$ is nonnegative, self-adjoint and has compact resolvent. \square

Our results from Section 2.1.2 and 2.1.1, that is Proposition 2.8 and Proposition 2.16, now imply the following corollary

Corollary 3.5 (Spectra of Interval Laplacians). *The spectra $\sigma(-\Delta^D)$ and $\sigma(-\Delta^N)$ satisfy*

$$\begin{aligned} [0, \infty) \supset \sigma(-\Delta^D) &= \{\lambda_i^D : i \in \mathbb{N}\} \quad \text{with } \lim_{i \rightarrow \infty} \lambda_i^D = \infty \\ [0, \infty) \supset \sigma(-\Delta^N) &= \{\lambda_i^N : i \in \mathbb{N}\} \quad \text{with } \lim_{i \rightarrow \infty} \lambda_i^N = \infty \end{aligned}$$

where $\sigma(-\Delta^D) = \sigma_p(-\Delta^D)$ and $\sigma(-\Delta^N) = \sigma_p(-\Delta^N)$ and all eigenvalues λ_i^D, λ_i^N have finite multiplicities.

3.1.2 Quantitative analysis

It is an easy task to actually compute the eigenvalues, which we will do in this short subsection. The results will illustrate the qualitative characterizations we developed in the preceding subsection.

We note the following elementary result.

Proposition 3.6. *Let $l := b - a$ then the eigenvalues and eigenfunctions of the Dirichlet and Neumann Laplacian, as presented in Problem 3.1, are given by ($\alpha \in \mathbb{R} \setminus \{0\}$)*

$$\begin{aligned} \sigma(-\Delta^D) &= \{(l^{-1}k\pi)^2 : k \in \mathbb{N}\} & \sigma(-\Delta^N) &= \{(l^{-1}k\pi)^2 : k \in \mathbb{N}_0\} \\ u_k^D(x) &= \alpha \sin(\sqrt{\lambda_k}x) & u_k^N(x) &= \alpha \cos(\sqrt{\lambda_k}x). \end{aligned}$$

Proof. We begin with the Dirichlet Laplacian. First, consider the case $\lambda = 0$, hence $-u'' = 0$. The general solution is given by $u(x) = ax + b$ with $a, b \in \mathbb{C}$, and the boundary conditions lead to $a = b = 0$. We hence end up with the trivial solution, which implies by definition that $0 \notin \sigma(-\Delta^D)$. Considering $\lambda > 0$ we obtain the general solution $u(x) = a \sin(\sqrt{\lambda}x) + b \cos(\sqrt{\lambda}x)$, and the boundary conditions lead to $b = 0$ and $\lambda = (l^{-1}k\pi)^2$ for $k \in \mathbb{N}$.

We continue with the Neumann Laplacian. The case $\lambda = 0$ with general solution $u(x) = ax + b$ with $a, b \in \mathbb{C}$ implies that $u(x) = b$ with $b \neq 0$ is an eigenfunction. Hence this time $0 \in \sigma(-\Delta^N)$. Now for $\lambda > 0$ we have again the general solution $u(x) = a \sin(\sqrt{\lambda}x) + b \cos(\sqrt{\lambda}x)$, and the boundary conditions result in $a = 0$ and $\lambda = (l^{-1}k\pi)^2$ for $k \in \mathbb{N}$. \square

3.1.3 Spectral comparison

Before we compare the spectra, we want to stress, that the Dirichlet and Neumann boundary conditions can be interpreted in the the frame of Kirchhoff and Anit-Kirchhoff conditions, as they have been introduced in Section 2.3. Indeed, considering the Dirichlet boundary conditions, we see that the sums of function values at the boundary equal zero, while the first derivative is continuous. The converse is true, when we consider the Neumann conditions. We hence see, that we can refer to the Dirichlet conditions as Anti-Kirchhoff, and to the Neumann conditions as Kirchhoff conditions.

Now we turn to the spectra. First, we see that the quantitative result, Proposition 3.1.2, is consistent with the quantitative result, Corollary 3.5. Moreover, a comparison of both spectra shows that they are not identical, but only differ in $\sigma(-\Delta^N)$ not including the 0. Later, in Section 3.2.4 we will interpret this difference from a broader perspective.

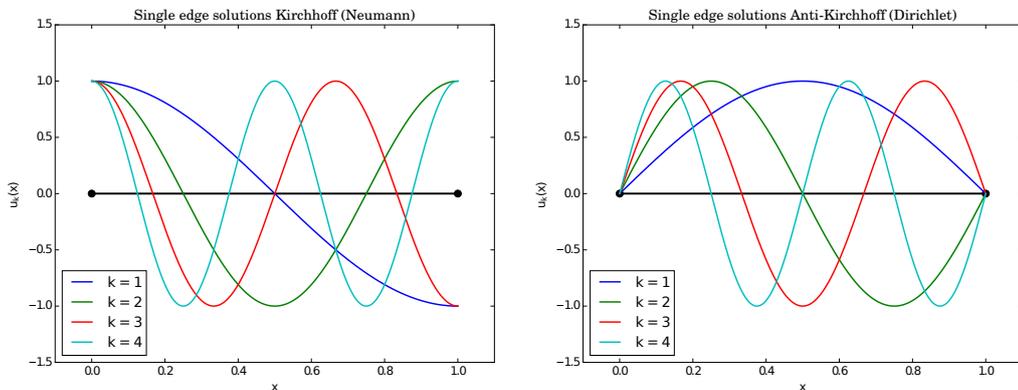


Figure 1: Some eigensolutions for Kirchhoff and Anti-Kirchhoff conditions

3.2 The standard Laplacian on finite equilateral quantum graphs

In this section we analyze compact quantum graphs under Kirchhoff and Anti-Kirchhoff conditions, where the respective Hamiltonian is taken from Definition 2.45. As in the section before we will at first derive a qualitative description of the spectra, followed by a quantitative consideration and a spectral comparison. Main sources have been [BK13, Section 1.4] and [vB85, Section 5].

In order to provide a clear formulation of the problem with all assumptions and notations we summarize the problem below.

Problem 3.7. *Let $\Gamma = (V, E)$ be a nonempty, connected, finite and simple combinatorial digraph with the vertex set $V = \{v_1, \dots, v_n\}$, the edge set $E = \{e_1, \dots, e_N\}$, the adjacency matrix $\mathcal{A}(\Gamma) = (e_{ij})$ and the signed incidence matrix $\mathcal{D}(\Gamma) = (d_{ij})$.*

We assume that Γ is equipped with a equilateral metric structure, meaning that each edge $e = (u, v) \in E$ is identified with the real interval $[0, 1]$ and an own coordinate $x_e \in [0, 1]$, where $x_e = 0$ and $x_e = 1$ correspond to u and v respectively. Finally on each edge $e_i \in E$ we define a corresponding edge-function by $u_i : [0, 1] \rightarrow \mathbb{R}, x \mapsto u_i(x)$.

We now want to find functions $u \in \bigoplus_{e \in E} H^2(e)$ that satisfy the Kirchhoff or Anti-Kirchhoff conditions, as well as scalars $\lambda \in \mathbb{C}$ such that $u|_{e_i} = u_i$ while $-u'_i = \lambda u_i$ for all $i \in \{1, \dots, N\}$. In operator notation these problems read: find $u \in \tilde{H}_{CK}^2(\Gamma)$ and $\bar{u} \in \tilde{H}_{KC}^2(\Gamma)$ such that

$$\begin{aligned} -\Delta_{\Gamma}^{CK} u &= \lambda u \\ -\Delta_{\Gamma}^{KC} \bar{u} &= \lambda \bar{u} \end{aligned}$$

3.2.1 Qualitative analysis

When we introduced the Hamiltonians $-\Delta_{\Gamma}^{CK}$ and $-\Delta_{\Gamma}^{KC}$ in Definition 2.45 we saw, that both of their domains were extensions from $\tilde{H}_0^2(\Gamma)$. The main result of this subsection, Theorem 3.12, is to show, that these extensions result in $-\Delta_{\Gamma}^{CK}$ and $-\Delta_{\Gamma}^{KC}$ being self-adjoint operators, where we follow the approach presented in [BK13, Section 1.4.1]. Before we get to this result, we need some preparations.

One of the central ideas in the proof of Theorem 3.12 is to consider each vertex of the underlying graph Γ independently. To do so, we are going to introduce some notation, that is convenient for that purpose, cf. [BK13, p. 16, 17].

Definition 3.8 (Vertex vectors). *Let (Γ_l, \mathcal{H}) be a compact quantum graph with graph $\Gamma_l = (V, E)$ and the associated signed incidence matrix $\mathcal{D}(\Gamma) = (d_{i,j})$. Let $v \in V$ and $E_v := \{e \in E : v \in e\} = \{e_1, \dots, e_k\}$ be the set of edges that contain v and f_1, \dots, f_k the corresponding edge-functions. We introduce the vertex-value vector F_v and the vertex-derivative vector F'_v as*

$$\begin{aligned} F_v &= (f_1(v), \dots, f_k(v))^T \\ F'_v &= (-d_{v,1}f_1(v), \dots, -d_{v,k}f_k(v))^T \end{aligned}$$

Note that the definition of F'_v is chosen, such that each entry of F'_v can be interpreted as an outgoing derivative at $v \in V$.

In the main proof of this subsection, the vertex conditions will be expressed in form of matrices with specific properties. In this context we will frequently use the following notation for concatenating matrices horizontally.

Definition 3.9. *Let $A \in \mathbb{C}^{n \times r}$ and $B \in \mathbb{C}^{n \times s}$ be two matrices with the same number of rows. We denote by $(A|B) \in \mathbb{C}^{n \times (r+s)}$ the matrix that results when concatenating A and B horizontally.*

We are now prepared to derive the first auxiliary result, see [BK13, Lemma 1.4.7].

Lemma 3.10. *Let $A, B \in \mathbb{C}^{n \times n}$ such that $(A|B)$ has full rank and AB^* is self-adjoint. Then for all $k \in \mathbb{R} \setminus \{0\}$ the matrix $A + ikB \in \mathbb{C}^{n \times n}$ has full rank and is thus invertible. Furthermore the matrix $M(k) := -(A + ikB)^{-1}(A - ikB)$ is unitary.*

Proof. We know from elementary linear algebra that for any complex valued matrix $T \in \mathbb{C}^{m \times n}$ we have the rank equality $\text{rank}(T) = \text{rank}(TT^*)$. By setting $T = A + ikB$ with $k \in \mathbb{R} \setminus \{0\}$ we obtain

$$\begin{aligned} \text{rank}(A + ikB) &= \text{rank}((A + ikB)(A + ikB)^*) \\ &= \text{rank}((A + ikB)(A^* - ikB^*)) \\ &= \text{rank}(AA^* + k^2BB^*) \\ &= \text{rank}((A|kB)(A|kB)^*) \\ &= \text{rank}((A|kB)) \\ &= \text{rank}((A|B)). \end{aligned}$$

Since $(A|B)$ has full rank, this shows the first part of the assertion. We move on to the second part. As we have just shown the matrix $A + ikB$ has full rank for real and non-zero k , and is thus invertible. The matrix $M(k) := -(A + ikB)^{-1}(A - ikB)$ is hence well-defined. To proof unitarity we need to show $M(k)M(k)^* = I = M(k)^*M(k)$. To that end reformulate $M(k)$ and obtain

$$\begin{aligned} M(k) &= -(A + ikB)^{-1}(A - ikB) \\ &= -(A + ikB)^{-1}(A - ikB)(A^* + ikB^*)(A^* + ikB^*)^{-1} \\ &= -(A + ikB)^{-1}(A + ikB)(A^* - ikB^*)(A^* + ikB^*)^{-1} \\ &= -(A^* - ikB^*)(A^* + ikB^*)^{-1} \end{aligned}$$

where we used $(A - ikB)(A^* + ikB^*) = (A + ikB)(A^* - ikB^*)$ which can easily be verified by a direct computation. We now use this result to check for unitarity.

$$\begin{aligned} M(k)M(k)^* &= -(A + ikB)^{-1}(A - ikB)(-(A^* - ikB^*)(A^* + ikB^*)^{-1})^* \\ &= (A + ikB)^{-1}(A - ikB)(A - ikB)^{-1}(A + ikB) = I \end{aligned}$$

Analogously we also obtain $M(k)^*M(k) = I$ which shows that $M(k)$ indeed is unitary. \square

Our next lemma is considering the embedding of $\tilde{H}^2(\Gamma)$ into $\tilde{L}^2(\Gamma)$. As in the case of a bounded one-dimensional interval, this embedding turns out to be compact as well.

Lemma 3.11. *Let $\Gamma_l = (\Gamma, l)$ be a compact metric graph, then $\tilde{H}^2(\Gamma) \xrightarrow{c} \tilde{L}^2(\Gamma)$.*

Proof. The Rellich-Kondrachov Theorem A.15 implies that $H^2(I) \xrightarrow{c} L^2(I)$ for a bounded one dimensional interval I , cf. Corollary 3.2. Therefore any sequence $(f_k)_{k \in \mathbb{N}} \subset H^2(I)$ with $\|f_k\|_{H^2} \leq 1$ for all $k \in \mathbb{N}$ contains a convergent subsequence $(f_{k_i})_{i \in \mathbb{N}}$ in $(L^2(I), \|\cdot\|_{L^2})$. Now consider a sequence $(f_k)_{k \in \mathbb{N}} := (f_k^{e_1}, \dots, f_k^{e_N})_{k \in \mathbb{N}} \subset \tilde{H}^2(\Gamma) = \bigoplus_{e_j \in E} H^2(e_j)$ with $\|f_k\|_{\tilde{H}^2} \leq 1$. With the compactness of Γ_l , and the above considered one dimensional case, it follows that $H^2(e_j) \xrightarrow{c} L^2(e_j)$ for all $j = 1, \dots, N$ which implies that $(f_k^{e_j})_{k \in \mathbb{N}}$ contains a convergent subsequence $(f_{k_i}^{e_j})_{i \in \mathbb{N}}$ in $(L^2(e_j), \|\cdot\|_{L^2})$ for all $j = 1, \dots, N$. We can hence find an increasing index sequence $(r_k)_{k \in \mathbb{N}} \subset \mathbb{N}$ such that $(f_{r_k}^{e_j})_{k \in \mathbb{N}}$ is convergent in $(L^2(e_j), \|\cdot\|_{L^2})$ for all $j = 1, \dots, N$, which implies that $(f_{r_k})_{k \in \mathbb{N}}$ is convergent in $(\tilde{L}^2(\Gamma), \|\cdot\|_{\tilde{L}^2})$. This shows $\tilde{H}^2(\Gamma) \xrightarrow{c} \tilde{L}^2(\Gamma)$ which is the assertion. \square

This already brings us to the main result of this subsection which gives a characterization of self-adjoint compact quantum graphs. The proof has been taken from [BK13, Theorem 1.4.4].

Theorem 3.12 (Self-adjoint extensions of compact quantum graphs). *Let $(\Gamma_l, -\Delta_\Gamma^{VC})$ be a compact quantum graph with combinatorial graph $\Gamma = (V, E)$ and Hamiltonian $-\Delta_\Gamma^{VC}$ defined by*

$$\begin{aligned} \tilde{H}_{VC}^2(\Gamma) &:= \{f \in \tilde{H}^2 : f \text{ satisfies the vertex conditions } VC\} \\ -\Delta_\Gamma^{VC} : \tilde{L}^2(\Gamma) &\supset \tilde{H}_{VC}^2(\Gamma) \rightarrow \tilde{L}^2(\Gamma) \\ f_e &\mapsto -f_e'' \text{ for all } e \in E \end{aligned}$$

where the function spaces $\tilde{L}^2(\Gamma)$ and $\tilde{H}_{VC}^2(\Gamma)$ are defined according to Definition 2.43. Then the following assertions are equivalent.

a) The Hamiltonian $-\Delta_\Gamma^{VC}$ is self-adjoint.

b) For every vertex $v \in V$ of degree γ_v there exist two matrices $A_v, B_v \in \mathbb{C}^{\gamma_v \times \gamma_v}$ such that $(A_v | B_v) \in \mathbb{C}^{\gamma_v \times 2\gamma_v}$ has maximal rank, $A_v B_v^*$ is self-adjoint and all $f \in \tilde{H}_{VC}^2(\Gamma)$ satisfy

$$A_v F_v + B_v F'_v = 0 \quad (5)$$

where the vertex vectors F_v and F'_v are defined as in Definition 3.8.

c) For every vertex $v \in V$ of degree γ_v there exists a unitary matrix $U_v \in \mathbb{C}^{\gamma_v \times \gamma_v}$ such that all $f \in \tilde{H}_{VC}^2(\Gamma)$ satisfy

$$i(U_v - I)F_v + (U_v + I)F'_v = 0. \quad (6)$$

d) For every vertex $v \in V$ of degree γ_v there exist three orthogonal (and also mutually orthogonal) projectors P_D^v, P_N^v and $P_R^v := I - P_D^v - P_N^v$, on \mathbb{C}^{γ_v} and an invertible self-adjoint operator Γ_v , acting on $P_R^v \mathbb{C}^{\gamma_v}$ such that all $f \in \tilde{H}_{VC}^2(\Gamma)$ satisfy

$$P_D^v F_v = 0 \quad (7a)$$

$$P_N^v F'_v = 0 \quad (7b)$$

$$P_R^v F'_v = \Lambda_v P_R^v F_v. \quad (7c)$$

Proof. To unburden the notation we will set $-\Delta := -\Delta_\Gamma^{VC}$ throughout this proof. We start with the assumption of self-adjointness from which we will work our way through the statements in the natural order $a) \Rightarrow b) \Rightarrow c) \Rightarrow d) \Rightarrow a)$.

a) \Rightarrow b) At first we assume that $-\Delta$ is self-adjoint (cf. Definition 2.15) on $\tilde{L}^2(\Gamma)$ with domain $\text{dom}(-\Delta) = \tilde{H}_{VC}^2(\Gamma)$ as described above. We have to show that in this case, that - if we express the vertex conditions as described in b), using the matrices A_v, B_v for $v \in V$ - these matrices have the properties as stated in b). Since these conditions consider each vertex independently we can confine our analysis to a single vertex $v \in V$.

We hence pick a vertex $v \in V$ and consider a function $f \in \text{dom}(-\Delta)$. By the definition of $\text{dom}(-\Delta)$ this implies that f satisfies the vertex conditions VC as described in b), which means that we can find $A_v, B_v \in \mathbb{C}^{\gamma_v \times \gamma_v}$ such that

$$A_v F_v + B_v F'_v = 0$$

with the vertex vectors F_v and F'_v as described in Definition 3.8. We also chose another function $g \in \bigoplus_{e \in E_v} C^\infty(e) \subset \tilde{H}^2(\Gamma)$ of which we assume that it is non-zero in a small vicinity of v , and vanishes at all other vertices. What conditions does g have to satisfy to be in the domain of the adjoint operator $-\Delta^*$? We check the respective condition, cf. Definition 2.11. Via integration by parts (twice) we obtain

$$\begin{aligned} \langle -\Delta f, g \rangle &= - \sum_{e \in E_v} \int_e f_e''(x) \bar{g}_e(x) dx \\ &= - \sum_{e \in E_v} \int_e f_e(x) \bar{g}_e''(x) dx - \sum_{e \in E_v} f_e'(v) \bar{g}_e(v) + \sum_{e \in E_v} f_e(v) \bar{g}_e'(v) \\ &= \langle f, -\Delta g \rangle - \langle F'_v, G_v \rangle_{\mathbb{C}^{\gamma_v}} + \langle F_v, G'_v \rangle_{\mathbb{C}^{\gamma_v}} \end{aligned} \quad (8)$$

with $G_v = (g_1(v), \dots, g_{\gamma_v}(v))^T$ and $G'_v = (g'_1(v), \dots, g'_{\gamma_v}(v))^T$ and $\langle \cdot, \cdot \rangle_{\mathbb{C}^{\gamma_v}}$ being the canonical scalar product on \mathbb{C}^{γ_v} . In the following we omit the specific denotation of the scalar product, since it will always be clear which scalar product is considered. From the above computation resulting in (8), we conclude that for $g \in \text{dom}(-\Delta^*)$ the last term $\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle$ has to vanish. Assume that g satisfies this condition, that is $\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle = 0$ for all $f \in \text{dom}(-\Delta)$, then we have $\langle -\Delta f, g \rangle = \langle f, -\Delta g \rangle$ for all $f \in \text{dom}(-\Delta)$, which - according to Definition 2.11 - implies that $g \in \text{dom}(-\Delta^*)$. Since we assumed that $-\Delta$ is self-adjoint it follows $g \in \text{dom}(-\Delta^*) = \text{dom}(-\Delta)$

which in particular means

$$A_v G_v + B_v G'_v = 0.$$

We just showed that if $A_v F_v + B_v F'_v = 0$ then $\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle = 0$ for all $f \in \text{dom}(-\Delta)$ is equivalent to $A_v G_v + B_v G'_v = 0$. As our next step we will show that this implies that $(A_v|B_v)$ has full rank. To that end assume that for all $f \in \text{dom}(-\Delta)$, i.e., f satisfying $A_v F_v + B_v F'_v = 0$ we have $\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle = 0$. On one hand this implies that $(F_v, F'_v)^T \in \ker(A_v|B_v)$, meaning that $(F_v, F'_v)^T$ lies in a subspace with dimension $\dim \ker(A_v|B_v) = \gamma_v - n$ with $n \in \{0, 1, \dots, \gamma_v\}$. On the other hand, due to $\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle = 0$ for all such f results in $2\gamma_v - n$ conditions on $(G_v, G'_v)^T$, one for each dimension of $\ker(A_v|B_v)$, resulting in $(G_v, G'_v)^T$ lying in a subspace with dimension $2\gamma_v - (\gamma_v - n) = \gamma_v + n$. Since $-\Delta$ is self-adjoint the same holds if we switch the roles of f and g resulting in $n = 0$ and therefore

$$\dim \ker(A_v|B_v) = \gamma_v$$

which shows that $(A_v|B_v)$ has full rank - giving the first of the two conditions stated in a).

The second condition was the self-adjointness of the matrix $A_v B_v^*$. To show this we assume $f \in \text{dom}(-\Delta)$, i.e., $A_v F_v + B_v F'_v = 0$. Now we chose an arbitrary $h \in \mathbb{C}^{\gamma_v}$ and set $G_v := -B^* h$ and $G'_v := A^* h$. Note that we can easily construct a function $g \in \bigoplus_{e \in E_v} C^\infty(e)$ that satisfies these vertex conditions, since on each edge the value $g_e(v)$ and the derivative $g'_e(v)$ can be chosen independently of each other. We now see that

$$\begin{aligned} \langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle &= \langle F_v, A_v^* h \rangle - \langle F'_v, -B_v^* h \rangle \\ &= \langle A_v F_v, h \rangle + \langle B_v F'_v, h \rangle \\ &= \langle A_v F_v + B_v F'_v, h \rangle \\ &= 0 \end{aligned}$$

where we used $A_v F_v + B_v F'_v = 0$. Due to the self-adjointness of $-\Delta$ this implies that we also have $A_v G_v + B_v G'_v = 0$ which - by recalling $G_v = -B^* h$ and $G'_v = A^* h$ - leads to

$$(-A_v B_v^* + B_v A_v^*) h = 0.$$

Since $h \in \mathbb{C}^{\gamma_v}$ was chosen arbitrarily we conclude that $A_v B_v^* = B_v A_v^* = (A_v B_v^*)^*$ showing the self-adjointness of $A_v B_v^*$. This concludes the first of four implication we wanted to show.

b) \Rightarrow c) Now we assume that we can express the vertex conditions by a set of matrix pairs (A_v, B_v) having the properties stated in b). According to Lemma 3.10 the matrix $A_v + ikB_v$ is invertible for any real $k \neq 0$, hence we can consider the matrix $-2i(A_v + ikB_v)^{-1}$. After multiplying equation (5) with this matrix, and rearranging the terms in two different ways, we obtain

$$\begin{aligned} -2i(A_v + ikB_v)^{-1} A_v &= i(M(k) - I) \\ -2i(A_v + ikB_v)^{-1} B_v &= -\frac{1}{k}(M(k) + I) \end{aligned}$$

which already gives equation (6) by setting $k = -1$ and $U_v = M(-1)$.

c) \Rightarrow d) Since U_v is unitary we have $|\lambda| = 1$ for all $\lambda \in \sigma(U_v)$, thus the following construction makes sense: For each vertex $v \in V$ we define P_D^v, P_N^v to be the orthogonal projectors onto the eigenspaces of U_v that corresponds to the eigenvalues -1 and $+1$ respectively. Consequently $P_R^v := I - P_D^v - P_N^v$ projects on the eigenspace of the remaining eigenvalues of U_v . The definition of the projectors implies that all three of them commute with U_v , and of course also with I . Hence they also commute with $U_v \pm I$. Keeping this in mind when multiplying (6) with P_D^v and P_N^v respectively we obtain

$$\begin{aligned} i(U_v - I)P_D^v F_v + (U_v + I)P_D^v F'_v &= 0 \\ i(U_v - I)P_N^v F_v + (U_v + I)P_N^v F'_v &= 0. \end{aligned}$$

Since P_D^v corresponds to the eigenspace of -1 we conclude $(U_v - I)P_D^v = 0$. With an analog

argument we see that $(U_v + I)P_D^v = 0$, and hence

$$\begin{aligned} P_D^v F_v &= 0 \\ P_N^v F'_v &= 0. \end{aligned}$$

Now we consider the remanding P_R^v . When we denote by $(U_v + I)_R$ the restriction of $(U_v + I)$ to the eigenspace of the eigenvalues that are not ± 1 , i.e., the space $P_R^v \mathbb{C}^{\gamma_v}$, then $(U_v + I)_R$ is invertible. We multiply (6) with P_R^v and rearrange the equation resulting in

$$\begin{aligned} P_R^v F'_v &= -i(U_v + I)_R^{-1}(U_v - I)P_R^v F_v \\ &= \Lambda P_R^v F_v \end{aligned}$$

where we defined $\Lambda := -i(U_v + I)_R^{-1}(U_v - I)$. This matrix is invertible and self-adjoint on $P_R^v \mathbb{C}^{\gamma_v}$.

d) \Rightarrow a) In this last part of the proof we assume that $\tilde{H}_{VC}^2(\Gamma) := \{f \in \tilde{H}^2(\Gamma) : f \text{ satisfies (7)}\}$ and have to show that $-\Delta$ is self-adjoint. We will do so by showing $\text{dom}(-\Delta) = \text{dom}(-\Delta^*)$, that is $\text{dom}(-\Delta^*) = \tilde{H}_{VC}^2(\Gamma)$ as defined before. We begin with showing symmetry. To that end assume that f, g satisfy (7), that is

$$\begin{aligned} P_D^v F_v &= 0 & P_D^v G_v &= 0 \\ P_N^v F'_v &= 0 & P_N^v G'_v &= 0 \\ P_R^v F'_v &= \Lambda_v P_R^v F_v & P_R^v G'_v &= \Lambda_v P_R^v G_v. \end{aligned}$$

Setting $I = P_D^v + P_N^v + P_R^v$ and recalling that for an orthogonal projector P it holds $\langle Px, y \rangle = \langle x, Py \rangle$ for all x, y on the considered Hilbert space, as well as $\langle x, y \rangle = \langle Px, Py \rangle$ and $PP = P$ we find

$$\begin{aligned} \langle F'_v, G_v \rangle &= \langle F'_v, (P_D^v + P_N^v + P_R^v)G_v \rangle \\ &= \langle F'_v, P_D^v G_v \rangle + \langle P_N^v F'_v, G_v \rangle + \langle P_R^v F'_v, G_v \rangle \\ &= \langle \Lambda P_R^v F_v, P_R^v G_v \rangle. \end{aligned}$$

An analogous computations for $\langle F_v, G'_v \rangle$ yields the same result, that is $\langle F_v, G'_v \rangle = \langle \Lambda P_R^v F_v, P_R^v G_v \rangle$ and hence $\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle = 0$ which implies $\langle -\Delta f, g \rangle = \langle f, -\Delta g \rangle$, thus symmetry.

Until this point we only showed that $\text{dom}(-\Delta) \subset \text{dom}(-\Delta^*)$. To prove equality we assume $g \in \bigoplus_{e \in E_v} C^\infty(e) \subset \tilde{H}^2(\Gamma)$ such that g does not vanish only in a small vicinity of v , and $\langle -\Delta f, g \rangle = \langle f, -\Delta g \rangle$, that is

$$\langle F_v, G'_v \rangle - \langle F'_v, G_v \rangle = 0 \tag{9}$$

for all $f \in \tilde{H}_{VC}^2(\Gamma)$. We have to show that $g \in \tilde{H}_{VC}^2(\Gamma)$, meaning that g satisfies (7).

To that end we first note that we can express (7) by setting $A_v := P_D^v - \Lambda P_R^v$ and $B_v = P_N^v + P_R^v$ and writing $A_v F_v + B_v F'_v = 0$ for $f \in \tilde{H}_{VC}^2(\Gamma)$. This is a consequence from the three projectors being mutually orthogonal. Moreover by this definition we have $A_v B_v^* = B_v A_v^*$, that is $A_v B_v^*$ is self-adjoint.

Now we choose an arbitrary $h \in \mathbb{C}^{\gamma_v}$ and pick $f \in \tilde{H}^2(\Gamma)$ such that $F_v = -B_v^* h$ and $F'_v := A_v^* h$, then $f \in \tilde{H}_{VC}^2(\Gamma)$ since $A_v B_v^* = B_v A_v^*$. Plugging these values into (9) we obtain

$$0 = \langle -B_v^* h, G'_v \rangle - \langle A_v^* h, G_v \rangle = \langle -h, A_v G_v + B_v G'_v \rangle$$

which implies $A_v G_v + B_v G'_v = 0$ since h was chosen arbitrarily. With the above definition of the matrices A_v, B_v it follows, that g satisfies (7), thus $g \in \tilde{H}_{VC}^2(\Gamma)$. We conclude that $\text{dom}(-\Delta) = \text{dom}(-\Delta^*)$, showing that $-\Delta$ is self-adjoint. \square

With this characterization we are now in a position to show that the Kirchhoff and Anti-Kirchhoff conditions are in fact two examples for such self-adjoint boundary conditions. With respect to the definition of the CK- and KC-conditions in Subsection 2.3.2 it is easy to see, that

for given $v \in V$ the corresponding matrices $A_v, B_v \in \mathbb{C}^{\gamma_v \times \gamma_v}$ are given by

$$A_v^{CK} = B_v^{KC} = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \quad B_v^{CK} = A_v^{KC} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}$$

At first we have to consider the rank of $(A_v|B_v)$ which is obviously full in both cases. Next we check $A_v B_v^*$ for being a self-adjoint matrix. Since the result $A_v B_v^* = 0$ is in both cases the zero matrix which trivially is self-adjoint, we see that both the Kirchhoff and Anti-Kirchhoff conditions indeed result in self-adjoint Hamiltonians. We summarize this result.

Corollary 3.13 (Self-adjointness). *The Hamiltonians $-\Delta_\Gamma^{CK}$ and $-\Delta_\Gamma^{KC}$ from Definition 2.45 are self-adjoint.*

In the remainder of this subsection we will show that both Hamiltonians $-\Delta_\Gamma^{KC}$ and $-\Delta_\Gamma^{CK}$ are not only self-adjoint, but also are nonnegative and have compact resolvent. First we show nonnegativity for which we refer to [Kuc04, p. 15,16].

Proposition 3.14 (Nonnegativity). *The Hamiltonians $-\Delta_\Gamma^{CK}$ and $-\Delta_\Gamma^{KC}$ from Definition 2.45 are nonnegative.*

Proof. We begin with $-\Delta_\Gamma^{CK}$. Assume $f \in \tilde{H}^2(\Gamma)$ satisfying the vertex conditions. Integrating by parts leads to

$$\begin{aligned} \langle -\Delta_\Gamma^{CK} f, f \rangle &= \sum_{e \in E} - \int_{o_e}^{t_e} f''(x) \bar{f}(x) dx \\ &= \sum_{e \in E} \left\{ [-f'(x) \bar{f}(x)]_{o_e}^{t_e} + \int_{e \in E} |f'(x)|^2 dx \right\} \\ &= \sum_{e \in E} \int_{e \in E} |f'(x)|^2 dx > 0. \end{aligned} \tag{10}$$

The first part of the above summation in (10) vanishes due to the Kirchhoff-flow condition, and we see, that $-\Delta_\Gamma^{CK}$ is in fact nonnegative. If we consider our second operator $-\Delta_\Gamma^{KC}$ we obtain a similar result by an analogous computation. In this case the first summation term in (10) vanishes due to the Anti-Kirchhoff flow condition, i.e., $\sum_{e \in E_v} f(v) = 0$. Both operators are hence examples for self-adjoint nonnegative operators, which - including our considerations above - proves the assertion. \square

To show that both Hamiltonians also have compact resolvent, we will use Lemma 3.11 from above. The following proof was taken from [BK13, Theorem 3.1.1].

Theorem 3.15 (Compact resolvent). *The Hamiltonians $-\Delta_\Gamma^{CK}$ and $-\Delta_\Gamma^{KC}$ from Definition 2.45 have compact resolvent.*

Proof. Let $\lambda \in \rho(\mathcal{H})$ with $\mathcal{H} \in \{-\Delta_\Gamma^{CK}, -\Delta_\Gamma^{KC}\}$. Then the resolvent operator $(\lambda - \mathcal{H})^{-1}$ is a bounded operator from $\tilde{L}^2(\Gamma)$ to $\text{dom}(\mathcal{H}) \subset \tilde{H}^2(\Gamma)$. From Lemma 3.11 we know that $\tilde{H}^2(\Gamma) \xrightarrow{c} \tilde{L}^2(\Gamma)$ which shows that $(\lambda - \mathcal{H})^{-1}$ is a compact operator on $\tilde{L}^2(\Gamma)$. \square

Finally we summarize the above results. We see that we obtained the same qualitative result, as we already did for bounded intervals, see Corollary 3.5.

Corollary 3.16 (Spectra of graph Laplacians). *The spectra $\sigma(-\Delta_\Gamma^{CK})$ and $\sigma(-\Delta_\Gamma^{KC})$ satisfy*

$$\begin{aligned} [0, \infty) \supset \sigma(-\Delta_\Gamma^{CK}) &= \{\lambda_i^{CK} : i \in \mathbb{N}\} \quad \text{with } \lim_{i \rightarrow \infty} \lambda_i^{CK} = \infty \\ [0, \infty) \supset \sigma(-\Delta_\Gamma^{KC}) &= \{\lambda_i^{KC} : i \in \mathbb{N}\} \quad \text{with } \lim_{i \rightarrow \infty} \lambda_i^{KC} = \infty \end{aligned}$$

where $\sigma(-\Delta_\Gamma^{CK}) = \sigma_p(-\Delta_\Gamma^{CK})$ and $\sigma(-\Delta_\Gamma^{KC}) = \sigma_p(-\Delta_\Gamma^{KC})$ and all eigenvalues $\lambda_i^{CK}, \lambda_i^{KC}$ have finite multiplicities.

3.2.2 Quantitative analyses by adjacency calculus

From the qualitative results of the previous section we already know, that the spectra of both types of quantum graphs that we consider here are discrete subsets of the nonnegative real numbers with finite multiplicities. The central assumption we used to obtain this result was Γ being compact, that is Γ containing only a finite number of edges, all of which are of finite length. What we did not take into account was the specific structure of the graph, which is encoded in its adjacency matrix \mathcal{A} and its length matrix \mathcal{L} . In this section we will use this additional information to specifically compute the spectra and the corresponding eigenvectors. To that end we will utilize the so-called *adjacency calculus* that has been introduced by Joachim von Below in his dissertation from 1984 [vB84] and which he more compactly summarized in [vB85] or recently in [vBM13].

In the first two Subsection 3.2.2 and 3.2.2 we will consider compact quantum graphs subjected to Kirchhoff and Anti-Kirchhoff conditions respectively. These sections will contain the main ideas of and theorems the general approach and finally a quantitative description of the spectrum and the eigenvectors of such quantum graphs. In the following Subsection 3.2.4 both spectra are compared, and it is discussed how they are related to each other. Finally, in the last Subsection 3.2.5 we will consider four generic examples of quantum graphs, and compute and visualize the respective spectra together with the corresponding eigenvectors.

Quantum graphs under Kirchhoff conditions

In this subsection we will perform a quantitative analysis of the spectrum of $-\Delta_{\Gamma}^{CK}$ on a given graph $\Gamma = (V, E)$ as described in problem 3.7. Our approach will be as follows: we will transform the eigenvalue problem from the canonical edgewise formulation, as given below in (11), to a matrix differential equation with the vertex conditions expressed as algebraic matrix equations, see (15). This form has the advantage that it can be treated by standard techniques from the theory of ordinary differential equations. We will solve the problem in matrix form, obtaining eigenvalues and multiplicities that only depend on the adjacency structure of the underlying combinatorial graph. We begin with repeating the formulation of the eigenvalue problem in the conventional edgewise manner. Find $\lambda \in [0, \infty)$ (as we know from our results in Section 3.2.2) such that

$$-u_j'' = \lambda u_j \quad \text{for all } j \in \{1, \dots, N\} \quad (11a)$$

$$u_i(v) = u_j(v) \quad \text{for all } v \in e_i \cap e_j \quad (11b)$$

$$\sum_{j=1}^N d_{ij} u_j'(v_i) = 0 \quad \text{for all } i \in \{1, \dots, n\}. \quad (11c)$$

In this formulation we have N functions u_j , each one defined on an own edge e_j . For the matrix formulation of the problem we will arrange these function in a common matrix U as described by the next definition, cf. [vB85, Eq.(3)].

Definition 3.17. *In the situation of (11) we define the matrix valued function U using the components of the adjacency matrix $\mathcal{A} = (e_{ij})$ and the signed incidence matrix $\mathcal{D} = (d_{ij})$ as*

$$U := (u_{ij}) : [0, 1] \rightarrow \mathbb{C}^{n \times n} \text{ with } x \mapsto u_{ij}(x) := e_{ij} u_{s(i,j)} \left(\frac{1 + d_{i,s(i,j)}}{2} - x d_{i,s(i,j)} \right) \quad (12)$$

It might be helpful to re-check with Definition 2.31 to understand (12). We see from the above definition that the component functions u_{ij} of U are identical zero, whenever the respective entry in the adjacency matrix \mathcal{A} is zero. Furthermore it is easy to see that u_{ij} and u_{ji} are strongly related, as described by the next lemma.

Lemma 3.18. *In the situation given in Definition 3.17 we have*

$$U^*(x) = U(1 - x) \quad (13)$$

$$U'(x)^* = -U'(1 - x) \quad (14)$$

Proof. For non-adjacent v_i and v_j with $i, j \in \{1, \dots, n\}$ we have $e_{ij} = 0$ and also $e_{ji} = 0$. With (12) we hence see that in this case $u_{ij}(x)^* = u_{ji}(x) = 0$. If on the other hand v_i and v_j are adjacent and say $d_{i,s(i,j)} = 1$ we get $e_{ij} = e_{ji} = 1$ and $d_{j,s(j,i)} = -1$ by the definition of \mathcal{D} . Using again our definition (12) we obtain $u_{ij}(1 - x)^* = u_{ji}(x)$ which we can equivalently write

as $u_{ij}(x)^* = u_{ji}(1-x)$ if we denote the transformed variable again by x . The last case with $d_{i,s(i,j)} = -1$ is treated analogously, which in summary shows (13). Equation (14) on the other hand follows immediately by differentiating (13) component-wise. \square

We hence see that if a component u_{ij} (which corresponds to an actual edge) describes the function $u_{s(i,j)}$ on an interval starting at v_i and ending in v_j , the component u_{ji}^* describes the complex conjugate function $u_{s(i,j)}^*$ in reverse, starting at v_j and ending in v_i .

As a next step we now have to express the eigenvalue problem (11) using the function U from Definition 3.17. The first line (11a) can obviously be translated into $-U'' = \lambda U$. To translate the second line (11b) which expresses the continuity of the graph function u at the vertices, we observe that in the case of continuity of u we have $u_{ij}(0) = u_{s(i,j)}(v_i) = u(v_i)$. This means, that if we denote $\phi := (u(v_i))$ and $e := (1)$ we can express (11b) simply by $\exists \phi \in \mathbb{C}^n$ such that $U(0) = \phi e^* \cdot \mathcal{A}$, where the operation \cdot refers to the Hadamard product, see Definition B.6. Finally we conclude by similar considerations that we can express (11c) by summing up the rows in $U'(0)$, which we can write as $U'(0)e$, and require that each of these sums is zero, hence $U'(0)e = 0$. As we now translated all lines from our first formulation in (11) to a formulation using our new matrix U , we can reformulate our problem now. We want to find $\lambda \in [0, \infty)$ such that there exists a nontrivial matrix function $U = (u_{ij})$ with $e_{ij} = 0 \Rightarrow u_{ij} = 0$ (see Definition 3.17) and

$$-U'' = \lambda U \quad \text{Matrix differential equation} \quad (15a)$$

$$U(0) = \phi e^* \cdot \mathcal{A} \quad \text{Continuity condition} \quad (15b)$$

$$U'(0)e = 0. \quad \text{Kirchhoff flow condition} \quad (15c)$$

It is becoming apparent, that whenever we consider the vertex conditions, the matrices $U(0)$ and $U'(0)$ as well as the vector $(u(v_i))$ enter the equations. To simplify our notation we introduce the following abbreviations for these terms, where we already used $\phi := (u(v_i))$ above.

Definition 3.19. *In the context of Definition 3.17 and problem (15) we define*

$$\Phi := U(0) \quad \Psi := U'(0) \quad \phi := (u(v_i)).$$

As our next step we will provide the general solution of the matrix differential equation (15a), that is the solution that does not take into account the vertex conditions described by the equations (15b) and (15c). For this simple result we only need the theory of ordinary differential equations, since we can solve (15a) simply by solving for each component function, see [vB85, p.315].

Lemma 3.20 (General solution). *Let U be a nontrivial solution of (15a) corresponding to the eigenvalue λ . Then $\lambda \in [0, \infty)$ and U is of the form*

$$U(x) = \begin{cases} \Phi + x(\Phi^* - \Phi) & \text{if } \lambda = 0 \\ \cos(\sqrt{\lambda}x)\Phi + \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}\Psi & \text{if } \lambda > 0. \end{cases}$$

Proof. From our qualitative analyses in the last section, cumulating in Proposition 3.14, we know that all eigenvalues are real and lie in $[0, \infty)$. If we now first assume $\lambda = 0$, that is considering $U'' = 0$, we obtain - by considering each component separately - that all solutions are given by

$$U(x) = \Phi + xM \quad M \in \mathcal{M} \quad (16)$$

with $\mathcal{M} := \{M = (m_{ij}) \in \mathbb{C}^{n \times n} : e_{ij} = 0 \Rightarrow m_{ij} = 0\}$. Taking into account (13) we find by plugging $x = 1$ into (16) that $U(1) = \Phi^* = \Phi + M$ hence $M = \Phi^* - \Phi$ which gives the assertion for $\lambda = 0$. In the remaining case all solutions of $U'' = -\lambda U$ and their derivatives are given by

$$U(x) = \sin(\sqrt{\lambda}x)A + \cos(\sqrt{\lambda}x)B \quad A, B \in \mathcal{M} \quad (17)$$

$$U'(x) = \sqrt{\lambda} \cos(\sqrt{\lambda}x)A - \sqrt{\lambda} \sin(\sqrt{\lambda}x)B \quad A, B \in \mathcal{M}. \quad (18)$$

which is also an immediate consequence from considering each entry separately. Inserting $x = 0$ into (17) and (18) respectively yields $A = \sqrt{\lambda}^{-1}\Psi$ and $B = \Phi$, which gives assertion for $\lambda > 0$ and concludes the proof. \square

In the proof of Lemma 3.20 we encountered the matrix set \mathcal{M} consisting of all matrices that have the same zero-components as the adjacency matrix of the considered graph. In the following we will come across more such spaces, which will be presented in the next definition.

Definition 3.21 (\mathcal{M} -spaces). *Let Γ be a combinatorial graph as described in problem 3.7 with adjacency matrix $\mathcal{A} = (e_{ij})_{n \times n}$ and $e = (1)_{n \times 1}$. We define the three matrix spaces*

$$\begin{aligned}\mathcal{M}(\Gamma) &:= \{M = (m_{ij}) \in \mathbb{C}^{n \times n} : e_{ij} = 0 \Rightarrow m_{ij} = 0\} \\ \mathcal{M}^-(\Gamma) &:= \{M \in \mathcal{M}(\Gamma) : M^* = -M \text{ and } Me = 0\} \\ \mathcal{M}^+(\Gamma) &:= \{M \in \mathcal{M}(\Gamma) : M^* = M \text{ and } Me = 0\}.\end{aligned}$$

In the context of eigenvalue multiplicities we will need to know the dimensions of the two matrix spaces \mathcal{M}^- and \mathcal{M}^+ . It turns out that these dimensions are determined by the number of vertices and edges within the graph together with property of bipartiteness, cf. [vB85, p.320-322].

Lemma 3.22 (Dimensions of \mathcal{M} -spaces). *Consider the three \mathcal{M} -spaces described in Definition 3.21. Then the following dimension formulas hold.*

$$\begin{aligned}\dim(\mathcal{M}^-) &= N - n + 1 \\ \dim(\mathcal{M}^+) &= \begin{cases} N - n + 1 & \text{if } \Gamma \text{ is bipartite} \\ N - n & \text{if } \Gamma \text{ is not bipartite} \end{cases}\end{aligned}$$

Proof. We begin with the formula for \mathcal{M}^- . Consider the restriction of the mapping

$$T : \mathbb{R}^N \rightarrow \mathbb{R}^{n \times n}, \quad x := (x_k)_{N \times 1} \mapsto T(x) := (e_{ij} d_{i,s(i,j)} x_{s(i,j)})_{n \times n}$$

to $\ker(\mathcal{D})$, that is $T|_{\ker(\mathcal{D})}$. Here, as usual, $\mathcal{D} = (d_{ij})_{n \times N}$ is the signed incidence matrix of the considered graph Γ . While the definition of T , that uses the signed incidence matrix \mathcal{D} , ensures that for every $x \in \mathbb{R}^N$ we have $T^*(x) = -T(x)$, the restriction to the domain $\ker(\mathcal{D})$ provides $T(x)e = 0$ for all $x \in \ker(\mathcal{D})$. Hence $T(\ker(\mathcal{D})) \subseteq \mathcal{M}^-$. If on the other hand $M = (m_{ij})_{n \times n} \in \mathcal{M}^-$ is given, then the assumptions $e_{ij} = 0 \Rightarrow m_{ij} = 0$, $M^* = -M$ and $Me = 0$ require M to be of the form $(e_{ij} d_{i,s(i,j)} x_{s(i,j)})_{n \times n}$ for some $x = (x_k)_{N \times 1} \in \ker(\mathcal{D})$, and hence $\mathcal{M}^- \subseteq T(\ker(\mathcal{D}))$. This shows that \mathcal{M}^- is isomorphic to $\ker(\mathcal{D})$ which by Proposition 2.40 shows $\dim \mathcal{M}^- = \dim \ker(\mathcal{D}) = N - n + 1$.

We continue with the two formulas for \mathcal{M}^+ , beginning with the bipartite case. In this context we note that the rank of \mathcal{D} does not change when we alternate the directions of the graph. If we are now given a bipartite graph with $V = V_1 \cup V_2, V_1 \cap V_2 = \emptyset$ we can assign its directions in a way that that all origins lie in V_1 and all terminals V_2 . As a consequence the entries of any row in the respective signed incidence matrix \mathcal{D} have all the same sign, which results in $\ker(\mathcal{D}) = \ker(\mathcal{A})$. With analogous arguments as before we can now construct an isomorphism between $\ker(\mathcal{D})$ and \mathcal{M}^+ by considering the restriction of the mapping

$$S : \mathbb{R}^N \rightarrow \mathbb{R}^{n \times n}, \quad x := (x_k)_{N \times 1} \mapsto S(x) := (e_{ij} x_{s(i,j)})_{n \times n}$$

to $\ker(\mathcal{D})$, i.e., $S|_{\ker(\mathcal{D})}$. We hence see that also in this case we have $\dim \mathcal{M}^+ = \dim \ker(\mathcal{D}) = N - n + 1$, which shows the second formula of the assertion.

This brings us to the last case, that is the dimension formula of \mathcal{M}^+ for non-bipartite graphs. This part of the proof will require the most effort to show. At first, we consider the case $N = n$. As we know from Lemma B.14 this corresponds to Γ having exactly one cycle ζ . Since we additionally assume that Γ is not bipartite we conclude $\mathcal{A}(\zeta)e \neq 0$. We now assume that Γ is larger than ζ , i.e., Γ is not a pure cycle. For showing that in that case also $\mathcal{A}(\Gamma)e \neq 0$ we partition $\mathcal{A}(\Gamma)$ and e without limitation as in the following equation

$$\mathcal{A}(\Gamma)e = \begin{pmatrix} \mathcal{A}(\zeta) & \mathcal{A}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} \mathcal{A}(\zeta)e_1 + \mathcal{A}_{12}e_2 \\ \mathcal{A}_{21}e_1 + \mathcal{A}_{22}e_2 \end{pmatrix}.$$

Since Γ is unicyclic we can find a row in $(\mathcal{A}_{21} | \mathcal{A}_{22})$ that only contains one 1, which shows that $(\mathcal{A}_{21} | \mathcal{A}_{22})e \neq 0$ and $\mathcal{A}(\Gamma)e \neq 0$. This result combined with Γ being connected and $\mathcal{A}(\Gamma)e \neq 0$ shows

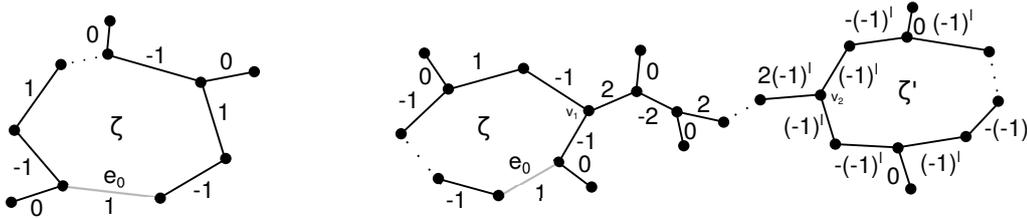


Figure 2: On the left side the first case, i.e., when Γ contains an even cycle - on the right side the opposite case, when Γ does not contain any even cycle. Note that the dashed lines indicate possible additional edges and not the removed edge. An example for an edge that we removed from the graph is colored gray.

that we cannot find a nontrivial matrix $M \in \mathcal{M}$ with $M = M^*$ and $Me = 0$ that is $\dim \mathcal{M}^+ = 0$. We hence see, that the dimension formula holds in the unicyclic case. In the following we can thus assume that Γ contains at least two cycles, which requires $N \geq 5$ edges. We will prove the dimension formula for these cases by induction over the number of edges N . Since we just showed the cases for $N < 5$ the induction base is given. Now assume that Γ has $N \geq 5$ edges, and that $\dim(\mathcal{M}^+) = N - n$ holds for any such graph with $\underline{N} < N$ edges. We will show that we can remove one of the N edges $e_0 \in E$ such that we obtain a connected and non-bipartite subgraph Γ_0 on the one hand, and on the other hand a matrix $M_0 \in \mathcal{M}^+$ that allows us to decompose \mathcal{M}^+ into the direct sum

$$\mathcal{M}^+(\Gamma) = \mathbb{R}M_0 \oplus \mathcal{M}^+(\Gamma_0).$$

Since in this case Γ_0 has $N - 1$ edges we can apply our induction hypothesis resulting at first in $\dim \mathcal{M}^+(\Gamma_0) = (N - 1) - n = N - n - 1$ and finally together with $\mathbb{R}M_0$ being one-dimensional in $\dim(\mathcal{M}^+) = N - n$. It remains to show that we actually can find such an edge $e_0 \in E$. For that purpose we distinguish two cases, both of which are visualized in figure 3.2.2.

First we assume that Γ contains an even cycle ζ , that is a cycle in Γ with an even number of edges $E(\zeta)$. In this case we can pick e_0 as one of the edges in $E(\zeta)$ that do not lie on all odd cycles of Γ . Such an edge obviously exists since ζ is even. Since the removed edge e_0 comes from a cycle, the resulting graph Γ_0 is connected. Also because ζ is even with e_0 not lying on all odd cycles, Γ_0 cannot turn out to be bipartite. We hence see, that Γ_0 satisfies the criteria. By assigning alternately ± 1 to the edges of ζ and 0 to the remaining edges of Γ , see figure 3.2.2, we define our matrix $M_0 \in \mathcal{M}(\Gamma)$ by writing these values to the respective entries. We see that in this manner each row of the symmetric matrix M_0 contains exactly one $+1$ and one -1 entry resulting in $M_0e = 0$. Since each matrix from $\mathcal{M}^+(\Gamma_0)$ has a zero-entry at the position of e_0 , we see that M_0 is indeed linear independent of $\mathcal{M}^+(\Gamma_0)$, which concludes the consideration for this case.

For the remaining case that Γ does not contain an even cycle, we choose two (odd) cycles ζ and ζ' where we pick any edge of ζ as e_0 . With the same argumentation as above we see that the resulting Γ_0 is connected and non-bipartite. Since Γ does not contain even cycles we conclude, that ζ and ζ' do not contain common edges - otherwise we could construct an even cycle using edges from both ζ and ζ' . We now consider a path Λ from an edge $v_1 \in \zeta$ to $v_2 \in \zeta'$ of length $l \geq 0$ with Λ having no common edges with ζ and ζ' respectively and assign values to the edges in the following manner: the two edges on ζ that contain v_1 are assigned with -1 , while the remaining edges in ζ are denoted with ± 1 alternately. The only edge on Λ that contains v_1 is assigned 2, while the following edges on Λ are assigned in turn $+2$ and -2 until $v_2 \in \zeta'$ is reached. The two edges on ζ' that contain v_2 are denoted with $(-1)^l$, and the remaining edges on ζ are alternating between $-(-1)^l$ and $(-1)^l$. One can now check, that this convention leads to a matrix $M_0 \in \mathcal{M}$ with $M_0e = 0$ and $M_0^* = M_0$, hence $M_0 \in \mathcal{M}^+$. Also, with the same arguments as in the case before, we see that M_0 is linear independent of $\mathcal{M}^+(\Gamma_0)$. This concludes the considerations for this last case, and thereby completes the proof. \square

Before we proceed with the quantitative discussion of the Kirchhoff spectrum, we still need one rather technical lemma in the context of Hadamard operations.

Lemma 3.23. Let $A = (a_{ij})_{m \times n}$ and $B = (b_{ij})_{m \times n} \in \mathbb{R}^{m \times n}$ and $x = (x_i)_{n \times 1} \in \mathbb{R}^n$ then

$$((A \cdot B)x)_i = (A \text{Diag}(x)B^T)_{ii}$$

Proof.

$$((A \cdot B)x)_i = \sum_{j=1}^n a_{ij} b_{ij} x_j = \sum_{j=1}^n a_{ij} x_j b_{ij} = (A \text{Diag}(x)B^T)_{ii}$$

□

This brings us to the main result of this subsection - the quantitative description of the spectrum for compact and equilateral quantum graphs under Kirchhoff conditions, see [vB85, p.317-323].

Proposition 3.24 (Kirchhoff spectrum). Let $(\Gamma_l, -\Delta_\Gamma^{CK})$ be a quantum graph under Kirchhoff conditions with transition matrix \mathcal{Z} as described in problem 3.7. Then its spectrum is given by

$$\sigma(-\Delta_\Gamma^{CK}) = \{0\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} \in \sigma(\mathcal{Z})\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} = -1\}$$

without counting multiplicities. The respective multiplicities ($m(\lambda) = 0$ is possible) are given by

$$m(\lambda) = \begin{cases} 1 & \text{if } \lambda = 0 \\ m(\cos \sqrt{\lambda}, \mathcal{Z}) & \text{if } \sin \sqrt{\lambda} \neq 0 \\ N - n + 2 & \text{if } \cos \sqrt{\lambda} = 1 \text{ and } \lambda > 0 \\ N - n + 2 & \text{if } \cos \sqrt{\lambda} = -1 \text{ and } \Gamma \text{ is bipartite} \\ N - n & \text{if } \cos \sqrt{\lambda} = -1 \text{ and } \Gamma \text{ is not bipartite.} \end{cases}$$

Proof. We start with the case $\lambda = 0$. From Lemma 3.20 we know that all solutions of (15a) with $\lambda = 0$, along with the respective derivatives are given by

$$U(x) = \Phi + x(\Phi^* - \Phi) \quad (19)$$

$$U'(x) = \Phi^* - \Phi. \quad (20)$$

We now easily get a new expression for Ψ by inserting $x = 0$ into (20) and using (15b)

$$\begin{aligned} \Psi &= \Phi^* - \Phi \\ &= (e\phi^* - \phi e^*) \cdot \mathcal{A}. \end{aligned} \quad (21)$$

Substituting (21) into the Kirchhoff flow condition (15c) and using Lemma 3.23 we compute

$$\begin{aligned} (\mathcal{A} \cdot e\phi^*)e &= (\mathcal{A} \cdot \phi e^*)e \\ \Rightarrow (\mathcal{A}\phi e^*)_{ii} &= (\mathcal{A}e\phi^*)_{ii} \\ \Leftrightarrow \mathcal{A}\phi &= \text{Diag}(\mathcal{A}e)\phi \\ \Leftrightarrow \text{Diag}(\mathcal{A}e)^{-1} \mathcal{A}\phi &= \phi \\ \Leftrightarrow \mathcal{Z}\phi &= \phi \end{aligned}$$

Hence the vertex distribution ϕ corresponding to the eigenvalue $\lambda = 0$ of (15) is an eigenvector of the transition matrix \mathcal{Z} belonging to the eigenvalue $\mu_1 = 1$, which is simple by Lemma 2.36.

We proceed with the second case, $\lambda > 0$, $\sin \sqrt{\lambda} \neq 0$. Referring again to Lemma 3.20, all these solutions, along with their respective derivatives, are of the form

$$U(x) = \cos(\sqrt{\lambda}x)\Phi + \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}\Psi \quad (22)$$

$$U'(x) = -\sqrt{\lambda} \sin(\sqrt{\lambda}x)\Phi + \cos(\sqrt{\lambda}x)\Psi \quad (23)$$

Plugging $x = 1$ into (22), using $U(1) = U^*(0) = \Phi^*$ from Lemma 3.18 and finally (15b) we obtain

$$\begin{aligned}
\Psi &= \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} (\Phi^* - \Phi \cos \sqrt{\lambda}) \\
&= \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} (e\phi^* - \cos \sqrt{\lambda} \phi e^*) \cdot \mathcal{A}
\end{aligned} \tag{24}$$

a new expression for Ψ . Substituting (24) into (15c) and using Lemma 3.23 we compute

$$\begin{aligned}
(e\phi^* \cdot \mathcal{A})e &= (\cos \sqrt{\lambda} \phi e^* \cdot \mathcal{A})e \\
\Rightarrow (\mathcal{A}\phi e^*)_{ii} &= \cos \sqrt{\lambda} (\mathcal{A}\phi^* e)_{ii} \\
\Leftrightarrow \sum_{j=1}^n a_{ij} \phi_i &= \cos \sqrt{\lambda} \phi_i \sum_{j=1}^n a_{ij} \\
\Leftrightarrow \mathcal{A}\phi &= \cos \sqrt{\lambda} \text{Diag}(\mathcal{A}e)\phi \\
\Leftrightarrow \mathcal{Z}\phi &= \cos \sqrt{\lambda} \phi
\end{aligned}$$

which shows the assertion for this case. For the remaining case of $\sin \sqrt{\lambda} = 0$ we will distinguish the cases $\cos \sqrt{\lambda} = 1$ and $\cos \sqrt{\lambda} = -1$. Note that in both cases due to Lemma 2.36 we have $\cos \sqrt{\lambda} \in \sigma(\mathcal{Z})$, which leaves us proving the multiplicity formulas only.

We will begin with the first case, i.e., assuming $\lambda > 0, \cos \sqrt{\lambda} = 1$. Considering the solutions space with vanishing Ψ we see from (22) and (15b) that every solution $U(x) = \cos(\sqrt{\lambda}x)\phi e^* \cdot \mathcal{A}$ is a multiple of \mathcal{A} giving this space only one dimension. If, on the other hand, we consider all solutions with vanishing Φ we obtain from $\Psi = -\Psi^*$ - this follows after plugging $x = 1$ into (23) - and (15c) that this solutions space is isomorphic to \mathcal{M}^- with $\dim(\mathcal{M}^-) = N - n + 1$, according to Lemma 3.22. Combining these results we obtain $m(\lambda) = N - n + 2$ as stated in the assertion.

For the remaining case $\lambda > 0, \cos \sqrt{\lambda} = -1$ we proceed in an analogous way. Again by plugging $x = 1$ into (23) we see that $\Psi = \Psi^*$ which together with (15c) indicates that the solution space with vanishing Φ is of dimension $\dim(\mathcal{M}^+)$ which, according to Lemma 3.22, is either $N - n + 1$ or $N - n$ depending on whether Γ is bipartite or not. For the solution space with vanishing Ψ we see again from (22) that this space is due to (15b), i.e., $\phi e^* \cdot \mathcal{A}$ at least one dimensional. By plugging $x = 1$ into (22) we see that $-\Phi^* = \Phi$ which is only possible for non-trivial Φ if Γ is bipartite, due to the continuity-condition (15b). If Γ is not bipartite we cannot label the vertices alternately with $+1$ and -1 without adjacent vertices getting the same value, which makes it impossible to construct a skew-symmetric matrix of the type $\phi e^* \cdot \mathcal{A}$. If we combine these results we obtain the remaining multiplicity formulas. \square

We see that the spectrum of the quantum graph $-\Delta_{\Gamma}^{CK}$ is tightly related to the transition matrix \mathcal{Z} of the underlying graph structure. If we want to compute the eigenvalues of a given quantum graph, as we consider them here, we first have to compute the eigenvalues of \mathcal{Z} . The specific formulas are given in the following corollary, which also states the corresponding eigenvectors.

Corollary 3.25 (Kirchhoff eigenvectors). *In the situation described in Proposition 3.24 we denote the eigenvalues of \mathcal{Z} by $1 = \mu_1 > \mu_2 > \dots > \mu_n \geq -1$ (see Lemma 2.36). Then the eigenvalues $\lambda_{r,k}$ ($k \in \mathbb{N}_0$) of the quantum graph $-\Delta_{\Gamma}^{CK}$ are given by*

$$\lambda_{r,k} = \begin{cases} 0 & \text{if } r = 1, k = 0 \\ (2k)^2 \pi^2 & \text{if } r = 1, k \neq 0 \\ (2k\pi \pm \arccos(\mu_r))^2 & \text{if } 1 < r < n \\ (2k+1)^2 \pi^2 & \text{if } r = n \text{ and } \Gamma \text{ is bipartite} \\ (2k\pi \pm \arccos(\mu_r))^2 & \text{if } r = n \text{ and } \Gamma \text{ is not bipartite} \\ (2k+1)^2 \pi^2 & \text{if } r = n+1 \text{ and } \Gamma \text{ is not bipartite} \end{cases}$$

Denoting with ζ_r the eigenvector of \mathcal{Z} corresponding to μ_r the eigenvectors $U_{r,k}(x)$ are given by

$$U_{r,k}(x) = \begin{cases} \alpha \mathcal{A} \cdot \zeta_1 e^* & \text{if } r = 1 \text{ and } k = 0 \\ \alpha \left(\cos(\sqrt{\lambda_{1,k}}x) \mathcal{A} + \frac{\sin(\sqrt{\lambda_{1,k}}x)}{\sqrt{\lambda_{1,k}}} \Psi \right) \text{ with } \begin{pmatrix} \Psi^* \\ \Psi_e \end{pmatrix} = \begin{pmatrix} -\Psi \\ 0 \end{pmatrix} & \text{if } r = 1 \text{ and } k \neq 0 \\ \alpha \left(\cos(\sqrt{\lambda_{r,k}}x) \zeta_r e^* + \frac{\sin(\sqrt{\lambda_{r,k}}x)}{\sin(\sqrt{\lambda_{r,k}})} (e \zeta_r^* - \cos(\sqrt{\lambda_{r,k}}) \zeta_r e^*) \right) \cdot \mathcal{A} & \text{if } 1 < r < n \\ \alpha \left(\cos(\sqrt{\lambda_{n,k}}x) \zeta_n e^* \cdot \mathcal{A} + \frac{\sin(\sqrt{\lambda_{n,k}}x)}{\sqrt{\lambda_{n,k}}} \Psi \right) \text{ with } \begin{pmatrix} \Psi^* \\ \Psi_e \end{pmatrix} = \begin{pmatrix} \Psi \\ 0 \end{pmatrix} & \text{if } r = n \text{ and } \Gamma \text{ bp} \\ \alpha \left(\cos(\sqrt{\lambda_{n,k}}x) \zeta_n e^* + \frac{\sin(\sqrt{\lambda_{n,k}}x)}{\sin(\sqrt{\lambda_{n,k}})} (e \zeta_n^* - \cos(\sqrt{\lambda_{n,k}}) \zeta_n e^*) \right) \cdot \mathcal{A} & \text{if } r = n \text{ and } \Gamma \text{ nbp.} \\ \alpha \left(\frac{\sin(\sqrt{\lambda_{n,k}}x)}{\sqrt{\lambda_{n,k}}} \Psi \right) \text{ with } \begin{pmatrix} \Psi^* \\ \Psi_e \end{pmatrix} = \begin{pmatrix} \Psi \\ 0 \end{pmatrix} & \text{if } r = n + 1 \end{cases}$$

As this corollary is a direct consequence of Proposition 3.24 we forgo a formal proof. The formula for the eigenvalues is obvious, and also all the eigenvectors already appear in the proof of Proposition 3.24. What remains to be shown is that all given eigenvectors above actually satisfy the eigenvalue problem 15, which is easy to check.

Quantum graphs under Anti-Kirchhoff conditions

In this subsection the quantitative analysis for our problem 3.7 with Anti-Kirchhoff vertex conditions is considered. The approach will be similar to the respective analysis for Kirchhoff conditions that has been presented in the preceding section. Some of the results we derived above can be reused in the context of Anti-Kirchhoff conditions, which makes this subsection shorter than the last one. We begin with stating problem 3.7 for the Anti-Kirchhoff case in the edgewise manner.

$$-u_j'' = \lambda u_j \quad \text{for all } j \in \{1, \dots, N\} \quad (25a)$$

$$d_{ki} u_i'(v_k) = d_{kj} u_j'(v_k) \quad \text{for all } v_k \in e_i \cap e_j \quad (25b)$$

$$\sum_{j=1}^N d_{ij}^2 u_j(v_i) = 0 \quad \text{for all } i \in \{1, \dots, n\} \quad (25c)$$

Using the same conventions as in the previous section, that is Definitions 3.17 and 3.19, we obtain the matrix differential equation for the Anti-Kirchhoff case. Since in this case the derivative u' is continuous on the graph, it makes sense to introduce the new abbreviation $\psi := (u'(v_i))$ which contains the derivatives evaluated at all vertices. Again we want to find $\lambda \in [0, \infty)$ such that there exists a nontrivial matrix function $U = (u_{ij})$ with $e_{ij} = 0 \Rightarrow u_{ij} = 0$ (see Definition 3.17) and

$$-U'' = \lambda U \quad \text{Matrix differential equation} \quad (26a)$$

$$U'(0) = \psi e^* \cdot \mathcal{A} \quad \text{Anti-Kirchhoff continuity condition} \quad (26b)$$

$$U(0)e = 0. \quad \text{Anti-Kirchhoff flow condition} \quad (26c)$$

We see that the roles of $U(0)$ and $U'(0)$ have changed if we compare (26) with (15). The following two propositions is the main result in the quantitative discussion of the spectrum for compact equilateral quantum graphs subjected to Anti-Kirchhoff conditions, cf. [vBM13, Theorem 3.5].

Proposition 3.26 (Anti-Kirchhoff spectrum). *Let $(\Gamma_l, -\Delta_\Gamma^{KC})$ be a quantum graph under Anti-Kirchhoff conditions with transition matrix \mathcal{Z} as in problem 3.7. Then the spectrum of $-\Delta_\Gamma^{KC}$ is given by*

$$\sigma(-\Delta_\Gamma^{KC}) = \{0\} \cup \{\lambda > 0 : -\cos \sqrt{\lambda} \in \sigma(\mathcal{Z})\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} = 1\}$$

without counting multiplicities. The respective multiplicities ($m(\lambda) = 0$ is possible) are given by

$$m(\lambda) = \begin{cases} N - n + 1 & \text{if } \lambda = 0 \text{ and } \Gamma \text{ is bipartite} \\ N - n & \text{if } \lambda = 0 \text{ and } \Gamma \text{ is not bipartite} \\ m(-\cos \sqrt{\lambda}, \mathcal{Z}) & \text{if } \sin \sqrt{\lambda} \neq 0 \\ N - n + 2 & \text{if } \cos \sqrt{\lambda} = -1 \\ N - n + 2 & \text{if } \cos \sqrt{\lambda} = 1, \lambda > 0 \text{ and } \Gamma \text{ is bipartite} \\ N - n & \text{if } \cos \sqrt{\lambda} = 1, \lambda > 0 \text{ and } \Gamma \text{ is not bipartite.} \end{cases}$$

Proof. We start with the first case $\lambda = \mathbf{0}$. As we know from Lemma 3.20 all solutions of the matrix differential equation (26a) for $\lambda = 0$ are given by $U(x) = \Phi + (\Phi^* - \Phi)x$. We will now show that the Anti-Kirchhoff conditions lead to a vanishing slope matrix, i.e., $\Phi^* - \Phi = 0$. Using integration by parts we find

$$\begin{aligned} 0 &= \sum_{j=1}^N \int_0^1 u_j'' u_j \, dx_j \\ &= \sum_{j=1}^N [u_j' u_j]_0^1 - \sum_{j=1}^N \int_0^1 u_j'^2 \, dx_j. \end{aligned}$$

Expanding the first term results in

$$\begin{aligned} \sum_{j=1}^N [u_j' u_j]_0^1 &= \sum_{j=1}^N u_j'(1) u_j(1) - \sum_{j=1}^N u_j'(0) u_j(0) \\ &= \sum_{j=1}^N (+1) u_j'(1) u_j(1) + \sum_{j=1}^N (-1) u_j'(0) u_j(0) \\ &= \sum_{j=1}^N \sum_{v_i \in e_j} d_{ij} u_j'(v_i) u_j(v_i) \\ &= \sum_{i=1}^n \sum_{j=1}^{\gamma_{v_i}} d_{ij} u_j'(v_i) u_j(v_i). \end{aligned}$$

Considering a fixed vertex v_i the Anti-Kirchhoff conditions result in $d_{ij} u_j'(v_i) = d_{ik} u_k'(v_i)$ for all $j, k \in \{1, \dots, N\}$ with $v_i \in e_j \cap e_k$. Hence we can write $d_{ij} u_j'(v_i) =: u'(v_i)$ and extract that term from the sum. This results in

$$\begin{aligned} \sum_{j=1}^N [u_j' u_j]_0^1 &= \sum_{i=1}^n \sum_{j=1}^{\gamma_{v_i}} u'(v_i) u_j(v_i) \\ &= \sum_{i=1}^n u'(v_i) \underbrace{\sum_{j=1}^{\gamma_{v_i}} u_j(v_i)}_{=0} \end{aligned}$$

due to the Anti-Kirchhoff vertex condition (26b). And all together we obtain

$$0 = \sum_{j=1}^N \int_0^1 u_j'' u_j \, dx_j = - \sum_{j=1}^N \int_0^1 u_j'^2 \, dx_j \leq 0$$

which can only hold if $u_j' \equiv 0$ for all $j \in \{1, \dots, N\}$ hence $\Phi^* - \Phi = 0$ or $\Phi^* = \Phi$. From the last result and (26c) we see that $\Phi \in \mathcal{M}^+$ which implies that eigenspace for $\lambda = 0$ is isomorphic to \mathcal{M}^+ whose dimension is given by Lemma 3.22 to $\dim(\mathcal{M}^+) = N - n + 1$ for Γ being bipartite and $\dim(\mathcal{M}^+) = N - n$ for Γ not being bipartite.

We continue with the case $\lambda > \mathbf{0}$, $\sin \sqrt{\lambda} \neq \mathbf{0}$. Once again utilizing Lemma 3.20 we know that all solutions of (26a) and their derivatives for this case are given by

$$U(x) = \cos(\sqrt{\lambda}x) \Phi + \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} \Psi \quad (27)$$

$$U'(x) = -\sqrt{\lambda} \sin(\sqrt{\lambda}x) \Phi + \cos(\sqrt{\lambda}x) \Psi. \quad (28)$$

By plugging $x = 1$ into (28) and using (14) we arrive at a new expression for Φ in terms of Ψ .

$$\begin{aligned}
-\Psi^* &= -\sqrt{\lambda} \sin \sqrt{\lambda} \Phi + \cos \sqrt{\lambda} \Psi \\
\Leftrightarrow \Phi &= \frac{1}{\sqrt{\lambda} \sin \sqrt{\lambda}} (\cos \lambda \Psi + \Psi^*)
\end{aligned}$$

Now we use the vertex conditions (26c) and (26b). In the same manner as in proof 3.24 we obtain

$$\begin{aligned}
(\mathcal{A} \cdot e\psi^*)e &= -\cos \sqrt{\lambda} (\mathcal{A} \cdot \psi e^*)e \\
\Leftrightarrow \mathcal{Z}\psi &= -\cos \sqrt{\lambda} \psi
\end{aligned}$$

which shows the assertion for this case. We now consider the case $\sin \sqrt{\lambda} = 0$. Here we have to distinguish the cases $\cos \sqrt{\lambda} = -1$ and $\cos \sqrt{\lambda} = 1$. Note that in both cases due to Lemma 2.36 we have $\cos \sqrt{\lambda} \in \sigma(\mathcal{Z})$, which leaves us proving the multiplicity formulas only.

We will begin with the first case, i.e., $\lambda > \mathbf{0}, \cos \sqrt{\lambda} = -1$. By plugging $x = 1$ into (27)

$$U(1) = \Phi^* = \Phi \cos \sqrt{\lambda} + \sqrt{\lambda}^{-1} \sin(\sqrt{\lambda}) \Psi$$

we conclude, that in this case $\Phi^* = -\Phi$. Considering all solutions (27) with vanishing Ψ we conclude $m(\lambda) \geq N - n + 1$ by using (26c) and Lemma 3.22. If we consider all solutions with vanishing Φ on the other hand, then according to (27) these solutions are of the form

$$U(x) = \lambda^{-1} \sin(\sqrt{\lambda}x) \Psi$$

with $\Psi = \Psi^*$ by (28). Using (26b) we see that $\Psi = \psi e^* \cdot \mathcal{A}$ is a multiple of \mathcal{A} , hence $m(\lambda) = N - n + 2$.

Finally we assume $\lambda > \mathbf{0}, \cos \sqrt{\lambda} = 1$. Then by (28) and (26b) we have $-\Psi^* = \Psi = \psi e^* \cdot \mathcal{A}$, for which there are only non-trivial solutions if Γ is bipartite, because otherwise we cannot alternately assign $+1$ and -1 to the vertices without any adjacent vertices getting the same value, which permits to define a skew-symmetric matrix of the form $\psi e^* \cdot \mathcal{A}$. In that case this solutions space is one dimensional. Considering all solutions with vanishing Ψ we obtain $\Phi^* = \Phi$ by (27), and by (26b) and lemma (3.22) we see that $m(\lambda) \geq N - n + 1$ in the bipartite and $m(\lambda) \geq N - n$ in the non-bipartite case, which together amounts to the remaining multiplicity formulas. \square

Corollary 3.27 (Anti-Kirchhoff eigenvectors). *In the situation described in Proposition 3.24 we denote the eigenvalues of \mathcal{Z} by $1 = \mu_1 > \mu_2 > \dots > \mu_n \geq -1$ (see Lemma 2.36). Then the eigenvalues $\lambda_{r,k}$ ($k \in \mathbb{N}_0$) of the quantum graph $-\Delta_{\Gamma}^{CK}$ are given by*

$$\lambda_{r,k} = \begin{cases} (2k+1)^2 \pi^2 & \text{if } r = 1 \\ ((2k+1)\pi \pm \arccos(\mu_r))^2 & \text{if } 1 < r < n \\ ((2k+1)\pi \pm \arccos(\mu_r))^2 & \text{if } r = n \text{ and } \Gamma \text{ is not bipartite} \\ (2k)^2 \pi^2 & \text{if } r = n, k \neq 0 \text{ and } \Gamma \text{ is bipartite} \\ 0 & \text{if } r = n+1, k = 0 \\ (2k)^2 \pi^2 & \text{if } r = n+1, k \neq 0 \text{ and } \Gamma \text{ is not bipartite.} \end{cases}$$

Denoting with ζ_r the eigenvector of \mathcal{Z} corresponding to μ_r the eigenvectors $U_{r,k}(x)$ are given by

$$U_{r,k}(x) = \begin{cases} \alpha \left(\cos(\sqrt{\lambda_{1,k}}x) \Phi + \frac{\sin(\sqrt{\lambda_{1,k}}x)}{\sqrt{\lambda_{1,k}}} \zeta_1 e^* \right) \cdot \mathcal{A} \text{ with } \begin{pmatrix} \Phi^* \\ \Phi_e \end{pmatrix} = \begin{pmatrix} -\Phi \\ 0 \end{pmatrix} & \text{if } r = 1 \\ \alpha \left(\frac{\cos(\sqrt{\lambda_{r,k}}x) \zeta_r e^* + e \zeta_r^*}{\sqrt{\lambda_{r,k}} \sin(\sqrt{\lambda_{r,k}}x)} \cos(\sqrt{\lambda_{r,k}}x) + \frac{\sin(\sqrt{\lambda_{r,k}}x)}{\sqrt{\lambda_{r,k}}} \zeta_r e^* \right) \cdot \mathcal{A} & \text{if } 1 < r < n \\ \alpha \left(\frac{\cos(\sqrt{\lambda_{n,k}}x) \zeta_n e^* + e \zeta_n^*}{\sqrt{\lambda_{n,k}} \sin(\sqrt{\lambda_{n,k}}x)} \cos(\sqrt{\lambda_{n,k}}x) + \frac{\sin(\sqrt{\lambda_{n,k}}x)}{\sqrt{\lambda_{n,k}}} \zeta_n e^* \right) \cdot \mathcal{A} & \text{if } r = n \text{ and } \Gamma \text{ nbp.} \\ \alpha \left(\cos(\sqrt{\lambda_{n,k}}x) \Phi + \frac{\sin(\sqrt{\lambda_{n,k}}x)}{\sqrt{\lambda_{n,k}}} \zeta_n e^* \right) \text{ with } \begin{pmatrix} \Phi^* \\ \Phi_e \end{pmatrix} = \begin{pmatrix} \Phi \\ 0 \end{pmatrix} & \text{if } r = n, k \neq 0 \text{ and } \Gamma \text{ bp.} \\ \alpha \Phi \text{ with } \begin{pmatrix} \Phi^* \\ \Phi_e \end{pmatrix} = \begin{pmatrix} \Phi \\ 0 \end{pmatrix} & \text{if } r = n+1 \text{ and } k = 0 \\ \alpha \left(\cos(\sqrt{\lambda_{n,k}}x) \Phi \right) \text{ with } \begin{pmatrix} \Phi^* \\ \Phi_e \end{pmatrix} = \begin{pmatrix} \Phi \\ 0 \end{pmatrix} & \text{if } r = n+1 \text{ and } k \neq 0 \end{cases}$$

3.2.3 Quantitative analyses by the secular equation

In this section we want to present yet another approach - evolving around the so-called *secular equation* - to quantitatively determine the spectrum of the Hamiltonians $-\Delta_\Gamma^{CK}$ and $-\Delta_\Gamma^{VC}$, as described in Problem 3.7. In fact this approach, which was first introduced by J.-P. Roth, see [Rot84], in 1984, is even broad enough to also be applicable for all compact quantum graphs in general, that is we do not have to assume an equilateral metric structure. However, since the subject of this thesis is focused on equilateral, compact quantum graphs, we will mostly be concerned with this specific case. The following discussion is essentially based on [BK13, Section 2.1 and 3.7.1].

At first we will explain the main idea of the approach. Assume we had found a (nontrivial) solution $0 \neq f \in \tilde{H}_{VC}^2(\Gamma)$ and a positive $0 < \lambda \in \mathbb{R}$ such that $-\Delta_\Gamma^{VC} f = \lambda f$, where $-\Delta_\Gamma^{VC}$ represents either $-\Delta_\Gamma^{CK}$ or $-\Delta_\Gamma^{VC}$. Since it turns out to be convenient, for the rest of this section we will denote the eigenvalue λ in the form $\lambda = k^2$, which makes sense, since we know from the qualitative analyses in Section 3.2.1 that λ is always a nonnegative real number. We hence have

$$-\Delta_\Gamma^{VC} f = k^2 f. \quad (29)$$

How does the solution f look like? Since (29) implies that $f_e := f|_e$ satisfies $-f_e'' = k^2 f_e$ for all $e \in E$ we can express the restriction of f to any edge $e \in E$ of Γ as $f_e(x_e) = a_1 e^{-ikx_e} + a_2 e^{ikx_e}$, where x_e denotes the edge coordinate (according to the assigned direction of e), and $a_1, a_2 \in \mathbb{C}$ are constants accounting for the vertex conditions. We can hence say that f can be described on each edge $e \in E$ as a superposition of the so-called *plane waves* e^{-ikx_e} and e^{ikx_e} .

At this point, a new idea comes into play. So far, we have considered a metric graph - roughly speaking - as a set of one-dimensional edge-intervals that were glued together at the vertices. Each edge was thereby associated with exactly one distinct direction, that is the natural direction of the interval. However, the solution of the eigenvalue problem does not depend on the choice of this direction. The spectra do not change, if we switch the directions of an edge-interval on the metric graph. This is illustrated by the results of the last section, where the spectra are given as a function of the adjacency matrix \mathcal{A} but not of the signed incidence matrix \mathcal{D} which contains the directions. Motivated by this observation we will start to consider each edge as a two-way-street consisting of two directed edges, also called bonds, with opposite directions, see Figure 3. This two-way-picture is especially suited when we consider the edgewise solutions $f_e(x_e) = a_1 e^{-ikx_e} + a_2 e^{ikx_e}$ which consist of two components. If we now fix a vertex v of a given edge $e = \{v, v'\}$ and define the coordinate x_e^v as the edge coordinate originating in v we can think of the solution component $f_{e,v}^{in}(x_e^v) := a_1 e^{-ikx_e^v} = a_{b'} e^{ik(-x_e^v)}$ to be defined on the incoming bond b' , while the other component $f_{e,v}^{out}(x_e^v) := a_2 e^{ikx_e^v} = a_b e^{ikx_e^v}$ can be thought of to be defined on the outgoing bond b with respect to the considered vertex v . The edge solution f_e is then obtained by adding both components, that is $f_e = f_{e,v}^{in} + f_{e,v}^{out}$. In the perspective of this interpretation of the solution, the situations at the vertices can be seen a system of incoming and outgoing waves of the same wavelength.

The natural question that arises at this point is: what purpose serves this cumbersome construction? It allows us to introduce a concept that is referred to in the literature as *scattering*. Roughly speaking scattering describes how the solution distributes or scatters at the vertices of the graph, if we understand it in terms of incoming and outgoing waves, as we sketched it in the paragraph above. We will now explain this concept in more detail.

Consider a fixed vertex $v \in V$, a fixed incident edge $e \in E_v$ and a solution $0 \neq f$ of (29) that has a unit incoming component on e , and zero incoming components on $e' \in E_v \setminus \{e\}$, that is $f_{e,v}^{in}(x_e^v) = e^{-ikx_e^v}$ and $f_{e',v}^{in}(x_{e'}^v) = 0$ for all $e' \in E_v \setminus \{e\}$. We will call the corresponding solution $f^{(e)}$. In this context we now introduce the so-called local scattering matrix $\sigma^{(v)}$ at vertex v , cf. [BK13, p. 38].

Definition 3.28 (Local scattering matrix). *Let $f^{(e)} \in \tilde{H}_{VC}^2(\Gamma)$ be a solution of (29) with $f_{e,v}^{in}(x_e^v) = e^{-ikx_e^v}$ and $f_{e',v}^{in}(x_{e'}^v) = 0$ for all $e' \in E_v \setminus \{e\}$ as described before. Then the local scattering matrix $\sigma^{(v)} := (\sigma_{e,e'}^{(v)}) \in \mathbb{C}^{\gamma_v \times \gamma_v}$ at the considered vertex $v \in e$, where $e, e' \in E_v$ is defined by*

$$\begin{cases} f_e^{(e)}(x_e^v) = e^{-ikx_e^v} + \sigma_{e,e}^{(v)} e^{ikx_e^v} & \text{on } e \\ f_{e'}^{(e)}(x_{e'}^v) = \sigma_{e',e}^{(v)} e^{ikx_{e'}^v} & \text{on } e' \neq e. \end{cases}$$

$$\begin{aligned}
f_{e,v}^{in}(x_e^v) &= a_{b'} e^{-ikx_e^v} = a_{b'} e^{-ikL_e} e^{ikx_e^{v'}} = f_{e,v'}^{out}(x_e^{v'}) \\
f_{e,v}^{out}(x_e^v) &= a_b e^{ikx_e^v} = a_b e^{ikL_e} e^{-ikx_e^{v'}} = f_{e,v'}^{in}(x_e^{v'})
\end{aligned}$$

Figure 3: Interpretation of an undirected edge $e = \{v, v'\}$ as the combination of two directed edges $b = (v, v')$ and $b' = (v', v)$ with opposite directions. The two edge coordinates x_e^v and $x_e^{v'}$ originate in the vertices v and v' respectively.

Note that in order to describe the complete local scattering matrix $\sigma^{(v)}$ we have to consider the solutions $f^{(e)}$ for all $e \in E_v$. In the situation described in Definition 3.28 we have one incoming unit wave and $|E_v|$ outgoing waves with amplitudes $\sigma_{e,e'}^{(v)}$ at the considered vertex v . This situation can be understood as the scattering of the incoming wave at v to the outgoing waves.

Before we continue to extend the scattering approach on the whole graph, we will have a closer look on the local scattering matrix and present a few of its properties. The following lemma was taken from [BK13, Lemma 2.1.3].

Lemma 3.29. *In the situation described in Definition 3.28 the local scattering matrix $\sigma^{(v)}(k)$ is unitary and can be expressed as*

$$\sigma^{(v)}(k) = -(A_v + ikB_v)^{-1}(A_v - ikB_v) \quad (30)$$

where $A_v, B_v \in \mathbb{C}^{\gamma_v \times \gamma_v}$ are the matrices described in Theorem 3.12 that express the vertex conditions at the considered vertex $v \in V$.

Proof. With respect to Lemma 3.10, stating unitarity of $-(A_v + ikB_v)^{-1}(A_v - ikB_v)$, we only have to show that $\sigma^{(v)}(k)$ can actually be expressed in the form (30). To that end we consider the solution $f^{(e)}$ described in Definition 3.28 and determine the vertex value and the vertex derivative vector $F_v^{(e)}$ and $F_v'^{(e)}$, cf. Definition 3.8. Using Definition 3.28 we obtain

$$\begin{aligned}
F_v^{(e)} &= (\delta_{e',e} + \sigma_{e',e}^{(v)}(k)) \\
F_v'^{(e)} &= ik(-\delta_{e',e} + \sigma_{e',e}^{(v)}(k))
\end{aligned}$$

where $\delta_{e',e}$ denotes the Kronecker delta. If we repeat this definition for every $e \in E_v$, that is obtaining $F_v^{(e)}$ and $F_v'^{(e)}$ for each solution $f^{(e)}$, $e \in E_v$, and concatenate the resulting $F_v^{(e)}$ and $F_v'^{(e)}$ horizontally in the two matrices \mathbb{F}_v and \mathbb{F}_v' , then these matrices can be expressed as

$$\begin{aligned}
\mathbb{F}_v &= \mathbb{I} + \sigma^{(v)}(k) \\
\mathbb{F}_v' &= ik(-\mathbb{I} + \sigma^{(v)}(k))
\end{aligned}$$

where \mathbb{I} denotes the identity matrix. Since all solutions $f^{(e)}$ satisfy the vertex conditions it follows from $A_v \mathbb{F}_v + B_v \mathbb{F}_v' = 0$ that

$$A_v(\mathbb{I} + \sigma^{(v)}(k)) + B_v(ik(-\mathbb{I} + \sigma^{(v)}(k))) = 0$$

which we can solve for $\sigma^{(v)}(k)$ and obtain (30). Note that $(A_v + ikB_v)^{-1}$ is invertible for $k \neq 0$ by Lemma 3.10. \square

The last result allows us to compute the local scattering matrices for Kirchhoff and Anti-Kirchhoff vertex conditions which we will denote as $\sigma_{CK}^{(v)}$ and $\sigma_{KC}^{(v)}$ respectively. To that end let $\Gamma = (V, E)$ be the underlying combinatorial graph of a given compact quantum graph, and consider a vertex $v \in V$ with γ_v incident edges collected in E_v . We begin with the discussion of the Kirchhoff case. As we have seen in Lemma 3.29 $\sigma^{(v)}$ can be computed using the local vertex matrices $A_v, B_v \in \mathbb{C}^{\gamma_v \times \gamma_v}$ as introduced in Section 3.2.1. For convenience we restate them at this point one more time for the Kirchhoff case.

$$A_v^{CK} = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \quad B_v^{CK} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}$$

A direct computation of (30) for different values of $0 < k$ and γ_v leads to the assumption that $\sigma_{CK}^{(v)}(k) = 2\gamma_v^{-1} - \mathbb{E}$, where $\mathbb{E} = (1)_{\gamma_v \times \gamma_v}$. This assumption can easily be confirmed by checking

$$A_v^{CK} - ikB_v^{CK} = -(A_v^{CK} + ikB_v^{CK})(2\gamma_v^{-1} - \mathbb{E})$$

which is equivalent to $2\gamma_v^{-1} - \mathbb{E} = -(A_v^{CK} + ikB_v^{CK})^{-1}(A_v^{CK} - ikB_v^{CK})$ and avoids the computation of the inverse $(A_v + ikB_v)^{-1}$. In the same way we can compute the local scattering matrix $\sigma_{KC}^{(v)}$ for the Anti-Kirchhoff case. The respective matrices for the vertex conditions read

$$A_v^{KC} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix} \quad B_v^{KC} = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

It is easy to see that in this case we have $\sigma_{KC}^{(v)} = -\sigma_{CK}^{(v)}$ which we can confirm in the same way as in the Kirchhoff case before. We see that in both cases the local scattering matrices are independent of k . We summarize our results.

Corollary 3.30. *Let $(\Gamma_L, -\Delta_\Gamma^{VC})$ be a compact quantum graph with $-\Delta_\Gamma^{VC} \in \{-\Delta_\Gamma^{CK}, -\Delta_\Gamma^{KC}\}$. The the local scattering matrices $\sigma_{CK}^{(v)}$ and $\sigma_{KC}^{(v)}$ are given by*

$$\sigma_{CK}^{(v)}(k) = \sigma_{CK}^{(v)} = \frac{2}{\gamma_v} - \mathbb{E} \quad (31)$$

$$\sigma_{KC}^{(v)}(k) = \sigma_{KC}^{(v)} = \mathbb{E} - \frac{2}{\gamma_v}. \quad (32)$$

Since we will later compute the scattering matrices of some specific quantum graphs, see Section 3.2.5, we compute the local scattering matrices for the relevant cases of $\gamma_v \in \{1, 2, 3\}$:

$$\sigma_{CK}^{(v)} \stackrel{\gamma_v=1}{=} 1 \quad (33) \quad \sigma_{CK}^{(v)} \stackrel{\gamma_v=2}{=} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (35) \quad \sigma_{CK}^{(v)} \stackrel{\gamma_v=3}{=} \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{pmatrix} \quad (37)$$

$$\sigma_{KC}^{(v)} \stackrel{\gamma_v=1}{=} -1 \quad (34) \quad \sigma_{KC}^{(v)} \stackrel{\gamma_v=2}{=} \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad (36) \quad \sigma_{KC}^{(v)} \stackrel{\gamma_v=3}{=} \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix} \quad (38)$$

Note that the independence of both local scattering matrices $\sigma_{CK}^{(v)}$ and $\sigma_{KC}^{(v)}$ from k can be put in a more general context. It turns out, that $\sigma^{(v)}$ is independent of k if and only if the vertex conditions at v have no Robin part, that is $P_{R,v} = 0$, if we express the vertex conditions by using the orthogonal projectors $P_{D,v}$, $P_{N,v}$ and $P_{R,v}$ introduced in Theorem 3.12. The corresponding results can be found in [BK13, p. 38-41]. But since we only need the k -independence of $\sigma_{CK}^{(v)}$ and $\sigma_{KC}^{(v)}$ we forego these rather technical considerations at this point.

We will now proceed by extending the scattering concept from a single vertex $v \in V$ to the whole graph Γ . To that end let (f, k) be an eigenpair of $-\Delta_\Gamma^{VC} f = k^2 f$. Considering a fixed vertex $v \in V$ with incident edge $e = \{v, v'\} \in E_v$, the restriction of f to this edge can be generally expressed as

$$f_e(x_e^v) = \underbrace{a_b e^{ikx_e^v}}_{f_{e,v}^{out}(x_e^v)} + \underbrace{\bar{a}_{b'}}_{f_{e,v'}^{out}(x_e^{v'})} e^{ikx_e^{v'}} = a_b e^{ikx_e^v} + \underbrace{\bar{a}_{b'}}_{a_{b'}} e^{ikL_e} e^{-ikx_e^v}$$

where L_e denotes the length of the edge (which in our case is always one, but for now we will leave the notation in its general form). If we repeat that consideration for every edge $e \in E_v$ and summarize the coefficients a_b and $\bar{a}_b e^{ikL_e}$ in the vectors $\alpha = (a_b)$ and $\beta = (e^{ikL_e} \bar{a}_b)$ we can express the vertex value and the vertex derivative vector at v as $F_v = \alpha + \beta$ and $F'_v = ik(\alpha - \beta)$. Plugging these vectors in the vertex condition $A_v F_v + B_v F'_v = 0$ and rearranging leads to

$$\alpha^v = -(A_v + ikB_v)^{-1}(A_v - ikB_v)\beta^v \quad (39)$$

$$= \sigma^{(v)}(k)\beta^v \quad (40)$$

which shows that both coefficient vectors are related to each other by the local scattering matrix $\sigma^{(v)}(k)$. If we now apply this construction for each vertex $v \in V$, we can collect all resulting equations in a linear system. While doing so, we will notice, that each coefficient appears twice - once as the weight of an incoming wave and once as a weight of an outgoing wave. We will hence end up with a $2|E| \times |E|$ system, described by the following definition, see [BK13, p. 41, 42].

Definition 3.31 (Global scattering matrix). *Let $(\Gamma_L, -\Delta_\Gamma^{VC})$ be a quantum graph as described in Corollary 3.30 with local scattering matrices $\sigma^{(v)}$ for all $v \in V$. We define the global scattering matrix $S(k) = (s_{b',b}) \in \mathbb{C}^{2|E| \times |E|}$ by setting*

$$s_{b',b} = \delta_{t(b),v} \delta_{o(b'),v} \sigma_{b',b}^{(v)}$$

where b, b' refer to the bonds of the graph.

Taking a closer look on this slightly cryptic definition, we see that the global scattering matrix relates the vector of the solution coefficients $a_b, a_{b'}$ as in (39) to a weighted version of themselves. Indeed, if we define the vector $a \in \mathbb{C}^{2|E|}$ to be this coefficient vector (note that the actual order of the different $a_b, a_{b'}$ in a depends on how we labeled the bonds b, b' over the graph Γ , cf. Section 3.2.5), and if we define $L := \text{Diag}(l_b)$, where the order of the l_b on the diagonal of L corresponds to the order of the elements in a , we obtain

$$a = S(k)e^{ikL}a. \quad (41)$$

From this relation it becomes obvious that k^2 is an eigenvalue of problem (29) if and only if the coefficient vector a is an eigenvector of $S(k)e^{ikL}$. The corresponding eigenvector f is then described by the plane waves e^{-ikx_e} and e^{ikx_e} weighted accordingly with the coefficients contained in a . We emphasize this connection in an own theorem, cf. [BK13, Theorem 2.1.8].

Theorem 3.32 (Secular equation I). *Let $(\Gamma_L, -\Delta_\Gamma^{VC})$ be a compact quantum graph. Then $k^2 \in \mathbb{C} \setminus \{0\}$ is an eigenvalue of $-\Delta_\Gamma^{VC}$ if and only if k satisfies the so-called secular equation*

$$\det(\mathbb{I} - S(k)e^{ikL}) = 0 \quad (42)$$

where $L := \text{Diag}(l_b)$ is the diagonal length matrix as described before.

The secular equation allows us to determine the eigenvalues of a compact quantum graph with the exception $k^2 = 0$. This exception arises since in the case $k^2 = 0$ the edgewise solutions are not given anymore by a superposition of plane waves.

It turns out that we can obtain an even stronger assertion than given in Theorem 3.32 whenever the global scattering matrix $S(k)$ does not depend on k . As we have seen before $\sigma_{CK}^{(v)}$ and $\sigma_{KC}^{(v)}$ are k -independent, hence also the respective global scattering matrices S_{CK} and S_{KC} are independent of k . It thus makes sense for us, to consider this more powerful result, which is stated in Theorem 3.34. Before we get there, we need a preparing lemma, see [BK13, Lemma 3.7.2].

Lemma 3.33. *Let $U \in \mathbb{C}^{n \times n}$, $n \in \mathbb{N}$ be a unitary matrix. Moreover let $e^{i\theta(k)}$, $k \in \mathbb{R}$ be an eigenvalue of Ue^{ikL} with $L := \text{Diag}(l_i)$, $l_i > 0$ for all $i = 1, \dots, n$ corresponding to the normalized eigenvector $u(k)$ then*

$$\frac{d\theta(k)}{dk} = \langle u(k), Lu(k) \rangle \quad (43)$$

which especially implies that $\frac{d\theta(k)}{dk} > 0$.

Proof. First, note that Ue^{ikL} is unitary since U and e^{ikL} are unitary, hence it makes sense to consider its eigenvalues in the form $e^{i\theta(k)}$, $k \in \mathbb{R}$. From the unitarity it also follows that we can choose $\theta(k)$ to be a real function. Moreover the components of Ue^{ikL} are constant or exponential function, implying that Ue^{ikL} is analytic, and thereby that $\theta(k)$ is analytic. Summarizing: $\theta(k)$ can be chosen real analytic. This allows us to differentiate the eigenvalue equation

$$Se^{ikL}u(k) = e^{i\theta(k)}u(k) \quad (44)$$

with respect to k leading to

$$Se^{ikL}iLu(k) + Se^{ikL}u'(k) = i\frac{d\theta(k)}{dk}e^{i\theta(k)}u(k) + e^{i\theta(k)}u'(k). \quad (45)$$

We will now compute the inner product of (45) with (44), that is

$$\langle Se^{ikL}iLu(k) + Se^{ikL}u'(k), Se^{ikL}u(k) \rangle = \langle i\frac{d\theta(k)}{dk}e^{i\theta(k)}u(k) + e^{i\theta(k)}u'(k), e^{i\theta(k)}u(k) \rangle$$

which results in

$$\begin{aligned} \langle u(k), iLu(k) \rangle &= \langle u(k), i\frac{d\theta(k)}{dk}u(k) \rangle \\ \Leftrightarrow \langle u(k), Lu(k) \rangle &= \frac{d\theta(k)}{dk} \langle u(k), u(k) \rangle \end{aligned}$$

which is, taking into account the normalization of $u(k)$, the stated identity (43). Since this implies $l_{min} \leq \theta'_j(k)$ for all $j = 1, \dots, n$ with $l_{min} = \min\{l_1, \dots, l_n\}$ we obtain $0 < \theta'_j(k)$ since $l_1, \dots, l_n > 0$. This concludes the proof. \square

We can now state the improvement of Theorem 3.32, which shows that in the case of a k -independent global scattering matrix not only the roots of the secular equation relate to the eigenvalues of the quantum graph Hamiltonian, but also the multiplicities of the roots coincide with the multiplicities of the respective eigenvalues, cf. [BK13, Theorem 3.7.1].

Theorem 3.34 (Secular equation II). *Let $(\Gamma_l, -\Delta_{\Gamma}^{VC})$ be a compact quantum graph with a k -independent global scattering matrix. Then $k^2 \in \mathbb{C} \setminus \{0\}$ is an eigenvalue of $-\Delta_{\Gamma}^{VC}$ with multiplicity m_{k^2} if and only if k is a root of the secular equation (42) with the same multiplicity.*

Proof. From Theorem 3.32 we already know that $k^2 \in \mathbb{C} \setminus \{0\}$ is an eigenvalue of $-\Delta_{\Gamma}^{VC}$ if and only if it is a root of the secular equation (42). Thus we only have to show that also the multiplicities coincide. The assertion states that for $k_0 \in \mathbb{C} \setminus \{0\}$ such that $\det(\mathbb{I} - Se^{ik_0L}) = 0$ the multiplicity $m_{\chi}(\lambda_0)$ of the root $\lambda_0 := 1$ of the characteristic polynomial $\chi_{Se^{ik_0L}}(\lambda) = \det(\lambda - Se^{ik_0L})$ coincides with the multiplicity $m_f(k_0)$ of the root k_0 in $f(k) := \det(\mathbb{I} - Se^{ikL})$. To confirm that claim, we reformulate $f(k)$ as

$$f(k) = \det(\mathbb{I} - Se^{ikL}) = \prod_{j=1}^{2E} (1 - e^{i\theta_j(k)}) \quad (46)$$

where $e^{i\theta_j(k)}$ denote the eigenvalues of Se^{ikL} . Now assume that $k_0 \neq 0$ satisfies $f(k_0) = 0$, such that $\lambda_0 = 1$ is an eigenvalue of Se^{ik_0L} with multiplicity m . We have to show that $f^{(r)}(k_0) = 0$ for all $\mathbb{N} \ni r < m$ and $f^{(m)}(k_0) \neq 0$. To that end let J be the index set of the m eigenvalue indices with $e^{i\theta_{j_0}(k_0)} = 1$ for all $j_0 \in J$. Then we rewrite (46) as

$$f(k) = f_r(k) \prod_{j \in J} (1 - e^{i\theta_j(k)}) = f_r(k) f_1(k). \quad (47)$$

Note that in this representation $f_1(k_0) = 0$ and $f_r(k_0) \neq 0$. If we now consider the first m

derivatives of $f(k)$, we can express these as

$$f^{(r)}(k) = \sum_{j \in J} p_{r,j}(k)(1 - e^{i\theta_j(k)}), \quad 0 < r < m \quad (48)$$

$$f^{(m)}(k) = \sum_{j \in J} p_{m,j}(k)(1 - e^{i\theta_j(k)}) + f_r(k)(-i)^m \prod_{j \in J} \theta'_j(k) e^{ikL} \quad (49)$$

for some function $p_{r,j}(k)$ and $p_{m,j}(k)$ resulting while computing the derivatives. Note that the last stated summand in (49) results from $f_r(k)f_1^{(m)}(k)$. From (48) it is obvious that $f^{(r)}(k_0) = 0$ for all $\mathbb{N} \ni r < m$. And since $\theta'_j(k_0) > 0$ for all $j \in 1, \dots, 2|E|$ according to Lemma 3.33, and $f_r(k_0) \neq 0$, we conclude that $f^{(m)}(k_0) \neq 0$.

It remains to be shown that if $k_0 \in \mathbb{C} \setminus \{0\}$ is a root of f with multiplicity m that $\lambda_0 = 1$ is an eigenvalue of Se^{ikL} (which implies that k^2 is an eigenvalue of $-\Delta_\Gamma^{VC}$ by Theorem 3.32) with the same multiplicity. But this implication is also a consequence of (48) and (49). Indeed, assume that f has a root at $k_0 \neq 0$ with multiplicity m such that the index set J , described above, has $n \neq m$ elements. Then by (48) and (49) we conclude that f has a root at k_0 with multiplicity $n \neq m$ contradicting the assumption. We hence conclude $|J| = m$, from which we see that $\lambda_0 = 1$ is an eigenvalue of Se^{ikL} with multiplicity m . \square

3.2.4 Discussion and spectral comparison

In the last two sections we obtained precise descriptions of both spectra $\sigma(-\Delta_\Gamma^{CK})$ and $\sigma(-\Delta_\Gamma^{KC})$ using the numbers of vertices and edges, the eigenvalues of the transition matrix \mathcal{Z} and finally the global graph property of Γ being bipartite or not. This enables us to proceed with our third and final step of our analysis program, that is comparing both of these spectra.

Beforehand, however, we want to have another look on both of the spectra, and give a few remarks. First of all, it has to be noted, that $\sigma(-\Delta_\Gamma^{CK})$ and $\sigma(-\Delta_\Gamma^{KC})$ are obviously closely related. Leaving aside multiplicities for a moment, the only difference in the two formulas

$$\begin{aligned} \sigma(-\Delta_\Gamma^{CK}) &= \{0\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} \in \sigma(\mathcal{Z})\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} = -1\} \\ \sigma(-\Delta_\Gamma^{KC}) &= \{0\} \cup \{\lambda > 0 : -\cos \sqrt{\lambda} \in \sigma(\mathcal{Z})\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} = 1\}. \end{aligned}$$

is a sign change regarding the eigenvalues of \mathcal{Z} . This close relationship between the spectra results in a similar way of partitioning them. One refers to the eigenvalues $\lambda > 0$ with $|\cos \sqrt{\lambda}| = 1$ as the eigenvalues associated with the single edge problem, whereas the set of $\lambda > 0$ with $|\cos \sqrt{\lambda}| < 1$ is called the set of immanent eigenvalues. We can hence write

$$\begin{aligned} \sigma(-\Delta_\Gamma^{CK}) &= \{0\} \cup \sigma_s(-\Delta_\Gamma^{CK}) \cup \sigma_i(-\Delta_\Gamma^{CK}) \\ \sigma(-\Delta_\Gamma^{KC}) &= \{0\} \cup \sigma_s(-\Delta_\Gamma^{KC}) \cup \sigma_i(-\Delta_\Gamma^{KC}). \end{aligned}$$

with $\sigma_s(-\Delta_\Gamma) = \{k^2\pi^2 : k \in \mathcal{Z} \setminus \{0\}\}$ and $\sigma_i(-\Delta_\Gamma^{CK}) = \{(2k\pi \pm \arccos \alpha)^2 : \alpha \in \sigma(\mathcal{Z}) \setminus \{-1, 1\}\}$ and $\sigma_i(-\Delta_\Gamma^{KC}) = \{((2k+1)\pi \pm \arccos \alpha)^2 : \alpha \in \sigma(\mathcal{Z}) \setminus \{-1, 1\}\}$. An eigenvalue of the first kind, that is $\lambda \in \sigma_s$, corresponds to an eigensolution which can be thought of as the union of single edge solutions which satisfy the respective vertex conditions. An eigenvalue of the second type, that is $\lambda \in \sigma_i$ is strongly tight to the adjacency structure of the considered graph. The corresponding eigensolutions are more complex in the sense, that its restrictions to a single edge are not necessarily solutions of this single edge problem, cf. [vBM13, Remark 3.3, 3.6].

Keeping this spectral partition in mind, we now discuss a reasonable way to compare them both. The first way that comes to mind, is a comparison with respect to identity. That is asking: When are both spectra identical in terms of values and multiplicities? This question is answered by the following result, cf. [vBM13, Corollary 3.9].

Corollary 3.35. *The spectra of the operators $-\Delta_\Gamma^{CK}$ and $-\Delta_\Gamma^{KC}$ described in problem 3.7 coincide, counting multiplicities, if and only if Γ is both unicyclic and bipartite.*

Proof. At first we consider the case that Γ is unicyclic and bipartite. From Proposition 3.24 and 3.26 we know that $\lambda = 0$ is an eigenvalue of both operators with multiplicities $m^{CK}(\lambda) = 1$ and

$m^{KC}(\lambda) = N - n + 1$ since Γ is bipartite. Because Γ is also unicyclic, which by Lemma B.14 results in $N = n$, we conclude that $m^{KC}(\lambda) = 1 = m^{CK}(\lambda)$.

For the nonzero part of the spectrum we once again go back to Proposition 3.24 and 3.26 which state that these parts of the spectra can be expressed as

$$\begin{aligned}\sigma(-\Delta_{\Gamma}^{CK}) &= \{0\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} \in \sigma(\mathcal{Z})\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} = -1\} \\ \sigma(-\Delta_{\Gamma}^{KC}) &= \{0\} \cup \{\lambda > 0 : -\cos \sqrt{\lambda} \in \sigma(\mathcal{Z})\} \cup \{\lambda > 0 : \cos \sqrt{\lambda} = 1\}.\end{aligned}$$

From Proposition 2.37 we know, that the spectrum of \mathcal{Z} is symmetric with respect to 0 since Γ is bipartite, hence $\sigma(-\Delta_{\Gamma}^{CK}) \setminus \{0\} = \sigma(-\Delta_{\Gamma}^{KC}) \setminus \{0\}$ without counting multiplicities. To include the multiplicities we consider the respective formulas which are also given in the propositions 3.24 and 3.26. By again using the symmetry of $\sigma(\mathcal{Z})$ we see that these values also coincide, hence $\sigma(-\Delta_{\Gamma}^{CK}) \setminus \{0\} = \sigma(-\Delta_{\Gamma}^{KC}) \setminus \{0\}$ counting multiplicities. This shows the " \Rightarrow " direction of the assertion.

For the converse implication, we assume that both spectra coincide counting multiplicities. From Proposition 3.24 and 3.26, we conclude that \mathcal{Z} has to be symmetric with respect to 0, which by Proposition 2.37 implies that Γ is bipartite. Finally, from the $\lambda = 0$ case in proposition, 3.24 and 3.26, we conclude $n = N$, which by B.14 shows that Γ is unicyclic. This shows the " \Leftarrow " direction of the assertion, and concludes the proof. \square

This condition is very specific. Only if the considered graph Γ is both bipartite as well as unicyclic the two spectra are identical. This of course does not include the identity of the corresponding eigenvectors, but the spectra $\sigma(-\Delta_{\Gamma}^{CK})$ and $\sigma(-\Delta_{\Gamma}^{KC})$ coincide in values and multiplicities. Considering this result one might now ask to what extent we can reduce the assumptions on Γ and still get a general assertion regarding the comparison of both spectra. To that end we are going to order the eigenvalues of $-\Delta_{\Gamma}^{CK}$ and $-\Delta_{\Gamma}^{KC}$ in an ascending order, that is

$$\sigma(-\Delta_{\Gamma}^{CK}) = \{\lambda_0^{CK}, \lambda_1^{CK}, \dots\} \text{ such that } \lambda_j^{CK} \leq \lambda_{j+1}^{CK} \text{ for all } j \in \mathbb{N}_0 \quad (50a)$$

$$\sigma(-\Delta_{\Gamma}^{KC}) = \{\lambda_0^{KC}, \lambda_1^{KC}, \dots\} \text{ such that } \lambda_j^{KC} \leq \lambda_{j+1}^{KC} \text{ for all } j \in \mathbb{N}_0 \quad (50b)$$

where we allow multi-entries since we include the multiplicities in our considerations. From that perspective we can actually extend the result from Corollary 3.35, cf. [vBM13, Remark 3.11].

Corollary 3.36. *Let Γ be a bipartite graph as described in problem 3.7. If we order the eigenvalues of $-\Delta_{\Gamma}^{CK}$ and $-\Delta_{\Gamma}^{KC}$ like in (50), the following relations between λ_j^{CK} and λ_j^{KC} hold for $j \in \mathbb{N}_0$.*

$$\begin{aligned}\lambda_j^{CK} &\leq \lambda_j^{KC} && \text{if } \Gamma \text{ is a tree} \\ \lambda_j^{CK} &= \lambda_j^{KC} && \text{if } \Gamma \text{ is unicyclic} \\ \lambda_j^{CK} &\geq \lambda_j^{KC} && \text{if } \Gamma \text{ is multicyclic}\end{aligned}$$

Proof. Considering Proposition 3.24 and 3.26 we know that eigenvalues corresponding to the case $\lambda > 0$ with $\sin \sqrt{\lambda} \neq 0$ coincide counting multiplicities for both quantum graphs, since $\sigma(\mathcal{Z})$ is symmetric with respect to zero in the bipartite case. We therefore just have to consider the remaining eigenvalues. In the case that Γ is a tree, hence $N - n = -1$, we see that $\lambda = 0$ is not an eigenvalue for the Anti-Kirchhoff case (see Proposition 3.26). Taking into account that the multiplicities for the case $\cos \sqrt{\lambda} = \pm 1$ coincide this result in $\sigma(-\Delta_{\Gamma}^{KC}) = \sigma(-\Delta_{\Gamma}^{CK}) \setminus \{0\}$, and therefore shifts the spectrum to $\lambda_j^{CK} \leq \lambda_j^{KC}$. The second case is already given in Corollary 3.35. Finally, the multicyclic case (that is $N - n > 0$) follows by similar arguments as the tree case, only that we have now $m^{KC}(\lambda = 0) > m^{CK}(\lambda = 0) = 1$ which results in a spectral shift in the other direction. The combination of these results gives the assertion. \square

Considering the above result one might wonder if we can also find a global spectral inequality if we additionally drop the assumption of bipartiteness. It turns out, that such an inequality does not exist. A counter example is given in [vBM13, Example 3.12].

3.2.5 Spectral analysis of generic quantum graphs

In this subsection we want to illustrate the results we obtained during our spectral analyses. We will consider four generic graphs subjected to Kirchhoff and Anti-Kirchhoff conditions, and compute their spectra as well as some of their eigenvectors. Since the specific form of the eigenvectors (eigenfunctions) is sometime hard to imagine, and since there are only very few illustrations in the literature, we will plot some of the eigenvectors for both cases.

The last subsections have shown that the spectra of both types of quantum graphs as well as their similarity is determined by the properties of bipartiteness and the number of cycles of the underlying combinatorial graph structure. We therefore will consider four kinds of graphs where each one represents a different combination of these key properties. These graphs are summarized in the following table.

	bipartite	not bipartite
unicyclic		
not unicyclic		

Table 1: Overview of the considered graphs

Before we analyze these graph, we will fix the labeling of the vertices and bonds, so that it is easier to follow the construction of the given adjacency and scattering matrices. Note that the given labeling below is arbitrary. Spectra and eigenvectors, of course, do not depend on this choice. We could also have chosen any other labeling.

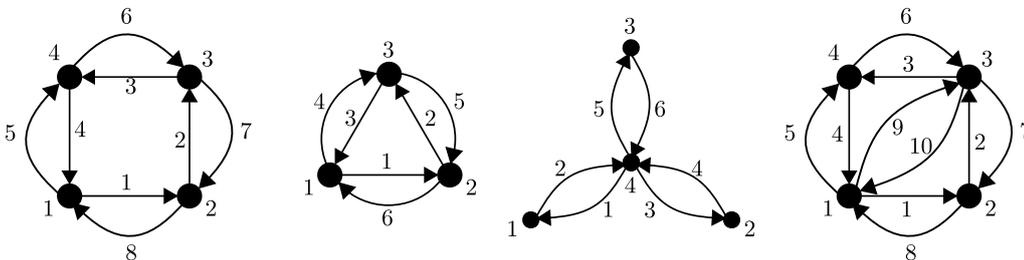


Figure 4: Labeling of vertices and bonds of the considered graphs

Bipartite and unicyclic We will walk through Table 1 from top to bottom and left to right. Hence, the first graph we consider is a cycle graph with four vertices and four edges ($n = 4, N = 4$), in graph theory referred to as C_4 . This graph is obviously unicyclic and bipartite, and thereby corresponds to the case where the spectra of $\sigma(-\Delta_{\Gamma}^{CK})$ and $\sigma(-\Delta_{\Gamma}^{KC})$ coincide, see Corollary 3.35. According to our vertex labeling form Figure 4 the adjacency matrix \mathcal{A} and the corresponding transition matrix \mathcal{Z} are given by

$$\mathcal{A} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad \mathcal{Z} = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}.$$

The eigenvalues of \mathcal{Z} counting multiplicities are given below. We also give the corresponding eigenvectors which we write in the columns of the matrix Σ . These eigenvectors are sorted according

to the order the eigenvalues are given in $\sigma(\mathcal{Z})$.

$$\sigma(\mathcal{Z}) = \{1, 0, 0, -1\} \quad \Sigma(\mathcal{Z}) = \begin{pmatrix} 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & -1 \end{pmatrix}$$

Considering Corollary 3.24 and 3.26 we are now able to compute the spectra. Before we do so, we want to introduce a specific notation that is used below. We set $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ and

$$\begin{aligned} \mathbb{N}^{(m)} &:= \underbrace{\{1, 1, \dots, 1\}}_{m \text{ times}}, \underbrace{\{2, 2, \dots, 2\}}_{m \text{ times}}, \{3, \dots\} \\ \mathbb{N}_0^{(m)} &:= \underbrace{\{0, 0, \dots, 0\}}_{m \text{ times}}, \underbrace{\{1, 1, \dots, 1\}}_{m \text{ times}}, \{2, \dots\}. \end{aligned}$$

The advantage of this notation is, as we will see below, that we can easily include the multiplicities of the respective eigenvalue sets in the following tables without needing extra columns. Also we use the abbreviation $\cos \sqrt{\lambda} > 0$ for $\cos \sqrt{\lambda}$ with $\lambda > 0$.

	Kirchhoff (CK)	Anti-Kirchhoff (KC)
$\lambda = 0$	$\{0\}$	$\{0\}$
$\cos \sqrt{\lambda} > 0 = 1$	$\{(2k)^2\pi^2 : k \in \mathbb{N}^{(2)}\}$	$\{(2k)^2\pi^2 : k \in \mathbb{N}^{(2)}\}$
$\sin \sqrt{\lambda} \neq 0$	$\{(2k\pi \pm \frac{\pi}{2})^2 : k \in \mathbb{N}_0^{(2)}\}$	$\{(2k\pi \pm \frac{\pi}{2})^2 : k \in \mathbb{N}_0^{(2)}\}$
$\cos \sqrt{\lambda} = -1$	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0^{(2)}\}$	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0^{(2)}\}$

Table 2: Comparison of the eigenvalues for C_4

Since C_4 has four vertices we find four roots μ_r of the transition matrix \mathcal{Z} . While μ_1 is always one (regardless of Γ), in this case we also have $\mu_n = \mu_4 = -1$ due to bipartiteness, and we see that the spectrum of \mathcal{Z} is therefore symmetric. The corresponding eigenvalues of the quantum graphs are the elements of $\sigma_s(-\Delta_\Gamma)$, i.e., the eigenvectors associated with the single edge problem. We find these values in the second and fourth line in Table 2 (not counting the very top line with the symbol and names). Between μ_1 and μ_n the spectrum of \mathcal{Z} has a double eigenvalue of $\mu_2 = \mu_3 = 0$, which corresponds to the immanent quantum graph spectra $\sigma_i(-\Delta)$, the values of which are given in the third row ($\cos \sqrt{\lambda} > 0$). If we order the eigenvalues in an ascending way and include their multiplicities, we obtain the following specific description of the spectra of both quantum graphs.

$$\begin{aligned} \sigma(-\Delta_\Gamma^{CK}) &= \left\{ 0, \left(\frac{\pi}{2}\right)^2, \left(\frac{\pi}{2}\right)^2, \pi^2, \pi^2, \left(\frac{3\pi}{2}\right)^2, \left(\frac{3\pi}{2}\right)^2, (2\pi)^2, (2\pi)^2, \left(\frac{5\pi}{2}\right)^2, \left(\frac{5\pi}{2}\right)^2, \dots \right\} \\ \sigma(-\Delta_\Gamma^{KC}) &= \left\{ 0, \left(\frac{\pi}{2}\right)^2, \left(\frac{\pi}{2}\right)^2, \pi^2, \pi^2, \left(\frac{3\pi}{2}\right)^2, \left(\frac{3\pi}{2}\right)^2, (2\pi)^2, (2\pi)^2, \left(\frac{5\pi}{2}\right)^2, \left(\frac{5\pi}{2}\right)^2, \dots \right\} \end{aligned}$$

Alternatively we could have also used the scattering approach to determine the spectra. To that end we have to construct the global scattering matrices for the Kirchhoff and Anti-Kirchhoff case for the considered graph C_4 . With respect to the labeling given in Figure 4 and taking into account the local scattering matrices (35) and (36) we obtain by Definition 3.31 the following global scattering matrices S_{CK} and S_{KC} alongside with the corresponding secular equation.

$$S_{CK} = -S_{KC} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

$$\begin{aligned} \det(\mathbb{I} - S_{CK}e^{ikL}) &= \det(\mathbb{I} - S_{KC}e^{ikL}) \\ &= (1 + e^{2ik})^2(1 + e^{ik})^2(-1 + e^{ik})^2 \end{aligned}$$

We see that this result corresponds with the eigenvalues given in Table 2 that have been computed using the adjacency calculus. We note, that also the multiplicities correspond to these in Table 2, as stated by Theorem 3.34.

Finally we want to consider the corresponding eigenvectors of some of the quantum graph eigenvalues. To that end we refer to Corollary 3.25 and Corollary 3.27. In Figure 5 below, the eigenvectors for all three types of eigenvalues have been plotted, that is eigenvectors associated with $\lambda = 0$, single-edge-problem-eigenvectors and finally eigenvectors corresponding to the immanent eigenvalues. Since the parameter $k \in \mathbb{N}$ from Table 2 only increases the number of periods in the respective harmonic functions, only the cases $k = 0$ and $k = 1$ have been considered. Note that the edge values (in the CK case) and the edge derivatives (in the KC case) correspond to the associated eigenvectors of the transition matrix \mathcal{Z} of the underlying graph.

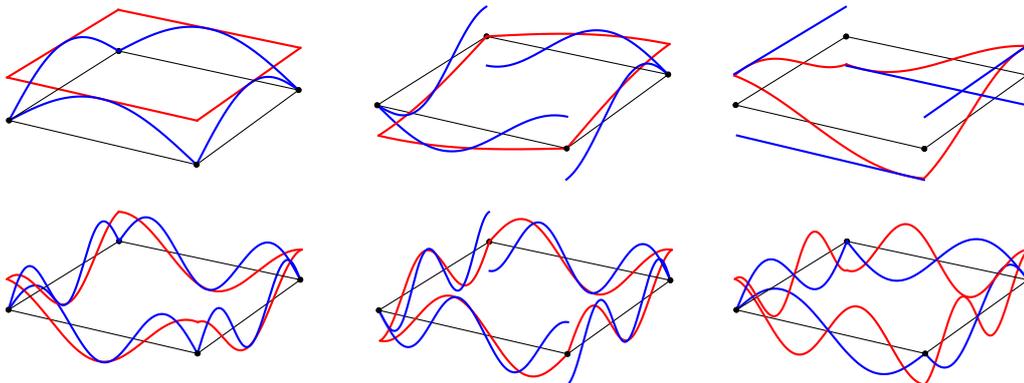


Figure 5: The C_4 eigenfunctions $U_{1,0}$ (top-left), $U_{2,0}$ (top-middle) and $U_{4,0}$ (top-right), as well as $U_{1,1}$ (bottom-left), $U_{2,1}$ (bottom-middle) and $U_{4,1}$ (bottom-right) for the CK case (red) and the KC case (blue), see Corollary 3.25 and Corollary 3.27.

Not bipartite but unicyclic If one removes one of the edges from the graph considered before (and connects the loose ends), the result is a graph that is still unicyclic but not bipartite anymore. This cycle graph with $n = 3$ and $N = 3$ is denoted as C_3 . As we know from Corollary 3.35 the spectra of $\sigma(-\Delta_{\Gamma}^{CK})$ and $\sigma(-\Delta_{\Gamma}^{KC})$ do not coincide in this case. This situation is illustrated below. First, we consider again the adjacency matrix \mathcal{A} and the transition matrix \mathcal{Z} (again with respect to Figure 4) of C_3 , together with the eigenvalues and eigenvectors of \mathcal{Z} (which are presented in the same way as we did it for C_4).

$$\mathcal{A} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad \mathcal{Z} = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$$

$$\sigma(\mathcal{Z}) = \left\{ 1, -\frac{1}{2}, -\frac{1}{2} \right\} \quad \Sigma(\mathcal{Z}) = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix}$$

Using Corollary 3.24 and 3.26 it is now possible to compute the spectra for both quantum graphs. The results are given in Table 3. As one can see on first sight, the spectra do not coincide indeed. The fact that C_3 is not bipartite results in $\lambda = 0$ not being an eigenvalue under Anti-Kirchhoff conditions anymore. Also, under Kirchhoff conditions we do not have anymore eigenvalues satisfying $\cos \sqrt{\lambda} = -1$. Considering the immanent eigenvalues we find $\sigma_i(-\Delta_\Gamma^{CK}) \cap \sigma_i(-\Delta_\Gamma^{KC}) = \emptyset$ which is a consequence of $\sigma(\mathcal{Z})$ not being symmetric anymore, which follows from Γ not being bipartite. An ascending ordering of both spectra, including multiplicities, leads to

$$\begin{aligned} \sigma(-\Delta_\Gamma^{CK}) &= \left\{ 0, \left(\frac{2\pi}{3}\right)^2, \left(\frac{2\pi}{3}\right)^2, \left(\frac{4\pi}{3}\right)^2, \left(\frac{4\pi}{3}\right)^2, (2\pi)^2, (2\pi)^2, \left(\frac{8\pi}{3}\right)^2, \left(\frac{8\pi}{3}\right)^2, \dots \right\} \\ \sigma(-\Delta_\Gamma^{KC}) &= \left\{ \left(\frac{\pi}{3}\right)^2, \left(\frac{\pi}{3}\right)^2, \pi^2, \pi^2, \left(\frac{5\pi}{3}\right)^2, \left(\frac{5\pi}{3}\right)^2, \left(\frac{7\pi}{3}\right)^2, \left(\frac{7\pi}{3}\right)^2, (3\pi)^2, (3\pi)^2, \dots \right\}. \end{aligned}$$

We see that in this case no general inequality like $\lambda_j^{CK} \leq \lambda_j^{KC}$ or $\lambda_j^{KC} \leq \lambda_j^{CK}$ holds, which is the result of C_3 not being bipartite.

Again we want to compare this result with the spectrum that we obtain by the scattering approach from Section 3.2.3. To deduce S_{CK} and S_{KC} we refer to the labeling given in Figure 4, and apply the construction given by Definition 3.31, and the local scattering matrices (35) and (36). We are led to the global scattering matrices S_{CK} and S_{KC} alongside with the corresponding secular equations as given below.

$$S_{CK} = -S_{KC} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\det(\mathbb{I} - S_{CK}e^{ikL}) = (e^{3ik} - 1)^2$$

$$\det(\mathbb{I} - S_{KC}e^{ikL}) = (e^{3ik} + 1)^2$$

which is in line with the results from the adjacency calculus result, given in Table 3.

Considering the eigenvectors of the quantum graphs, see Figure 3, the fact that C_3 is not bipartite results in no eigenvectors with an edge distribution - either with respect to the function values (CK), or with respect to the function derivatives (KC) - of only ± 1 values, where both signs appear at least once.

	Kirchhoff (CK)	Anti-Kirchhoff (KC)
$\lambda = 0$	$\{0\}$	\emptyset
$\cos \sqrt{\lambda} > 0 = 1$	$\{(2k)^2\pi^2 : k \in \mathbb{N}^{(2)}\}$	\emptyset
$\sin \sqrt{\lambda} \neq 0$	$\{(2k\pi \pm \frac{2\pi}{3})^2 : k \in \mathbb{N}_0^{(2)}\}$	$\{((2k+1)\pi \pm \frac{2\pi}{3})^2 : k \in \mathbb{N}_0^{(2)}\}$
$\cos \sqrt{\lambda} = -1$	\emptyset	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0^{(2)}\}$

Table 3: Comparison of the eigenvalues for C_3

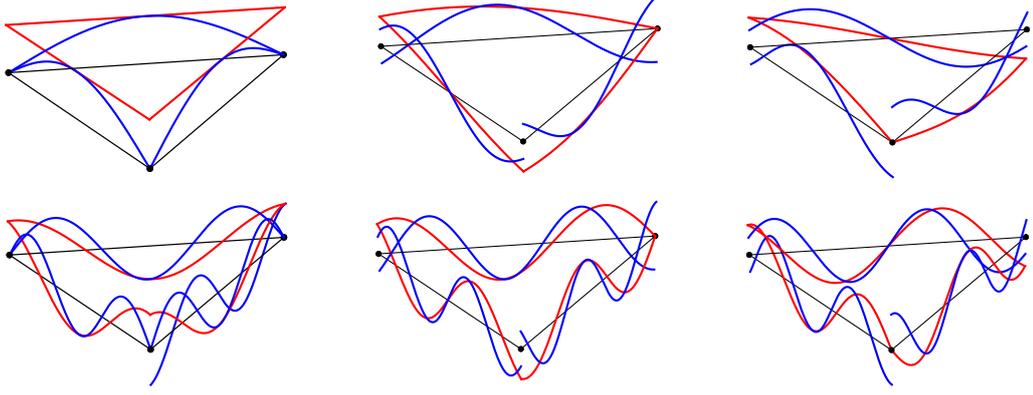


Figure 6: The C_3 eigenfunctions $U_{1,0}$ (top-left), $U_{2,0}$ (top-middle) and $U_{3,0}$ (top-right), as well as $U_{1,1}$ (bottom-left), $U_{2,1}$ (bottom-middle) and $U_{3,1}$ (bottom-right) for the CK case (red) and the KC case (blue), see Corollary 3.25 and Corollary 3.27.

Bipartite but not unicyclic The next graph is not a cycle graph anymore, but a star graph. It has four vertices and three edges ($n = 4, N = 3$), and graph theoretic literature refers to this graph as S_3 . Star graphs are always bipartite, but not unicyclic. According to our results above (Corollary 3.36), a general inequality with respect to the ordered eigenvalues of both quantum graphs (including multiplicities), that is $\lambda_j^{CK} \leq \lambda_j^{KC}$, can be made. We will see this result reflected in the results below. Before we get there, we will again give the adjacency matrix \mathcal{A} (according to the labeling presented in Figure 4), the transition matrix \mathcal{Z} and the eigenvalues and eigenvectors of \mathcal{Z} , as we did it for the examples above.

$$\mathcal{A} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \quad \mathcal{Z} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$$

$$\sigma(\mathcal{Z}) = \{1, 0, 0, -1\} \quad \Sigma(\mathcal{Z}) = \begin{pmatrix} 1 & -1 & \frac{1}{2} & 1 \\ 1 & 0 & -1 & 1 \\ 1 & 1 & \frac{1}{2} & 1 \\ 1 & 0 & 0 & -1 \end{pmatrix}.$$

Using the usual formulas from Corollary 3.24 and 3.26 in context with the approach using the adjacency calculus, we obtain the spectra given in Table 4. As we can see, the spectra do not coincide, but the difference is not too big. Indeed, the only mismatch is encountered for $\lambda = 0$, which is not contained in the Anti-Kirchhoff spectrum, but does appear in the Kirchhoff spectrum. For the remaining eigenvalues we have the same sets for both quantum graphs.

	Kirchhoff (CK)	Anti-Kirchhoff (KC)
$\lambda = 0$	$\{0\}$	\emptyset
$\cos \sqrt{\lambda} > 0 = 1$	$\{(2k)^2\pi^2 : k \in \mathbb{N}\}$	$\{(2k)^2\pi^2 : k \in \mathbb{N}\}$
$\sin \sqrt{\lambda} \neq 0$	$\{(2k\pi \pm \frac{\pi}{2})^2 : k \in \mathbb{N}_0^{(2)}\}$	$\{(2k\pi \pm \frac{\pi}{2})^2 : k \in \mathbb{N}_0^{(2)}\}$
$\cos \sqrt{\lambda} = -1$	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0\}$	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0\}$

Table 4: Comparison of the eigenvalues for S_3

As for the two examples before we also want to give an ordered spectrum for both $\sigma_i(-\Delta_\Gamma^{CK})$ and $\sigma_i(-\Delta_\Gamma^{KC})$ in this case. Taking into account the respective multiplicities we obtain

$$\begin{aligned}\sigma(-\Delta_\Gamma^{CK}) &= \left\{ 0, \left(\frac{\pi}{2}\right)^2, \left(\frac{\pi}{2}\right)^2, \pi^2, \left(\frac{3\pi}{2}\right)^2, \left(\frac{3\pi}{2}\right)^2, (2\pi)^2, \left(\frac{5\pi}{2}\right)^2, \left(\frac{5\pi}{2}\right)^2, \dots \right\} \\ \sigma(-\Delta_\Gamma^{KC}) &= \left\{ \left(\frac{\pi}{2}\right)^2, \left(\frac{\pi}{2}\right)^2, \pi^2, \left(\frac{3\pi}{2}\right)^2, \left(\frac{3\pi}{2}\right)^2, (2\pi)^2, \left(\frac{5\pi}{2}\right)^2, \left(\frac{5\pi}{2}\right)^2, \dots \right\}\end{aligned}$$

from which one can see that the general inequality $\lambda_j^{CK} \leq \lambda_j^{KC}$ holds. Since the only difference in the spectra lies in the eigenvalue zero, we expect that both secular equations - that is for the Kirchhoff case and the Anti-Kirchhoff case - will coincide. In order to check on that matter we derive the global scattering matrices (with respect to Figure 4 and taking into account the local scattering matrices (33), (34), (37) and (38)) and compute the secular equations. The results are presented below.

$$S_{CK} = -S_{KC} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & -\frac{1}{3} & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 & -\frac{1}{3} & 0 \end{pmatrix}$$

$$\begin{aligned}\det(\mathbb{I} - S_{CK}e^{ikL}) &= \det(\mathbb{I} - S_{KC}e^{ikL}) \\ &= -(1 + e^{ik})(-1 + e^{ik})(1 + e^{2ik})^2\end{aligned}$$

We see that the secular equations coincide indeed, and we also see that the roots are in line with the results from the adjacency calculus summarized in Table 4, including the multiplicities.

This brings us to the eigenvectors, see Figure 7. Since the considered graph is bipartite, the spectrum of \mathcal{Z} is symmetric, resulting in an eigenvector with a vertex value distribution (Kirchhoff) or a vertex derivative distribution (Anti-Kirchhoff) that contains only values of ± 1 where both signs appear at least once. Next to this bipartite-specific eigenvector, the plot below also contains two immanent eigenvectors in the center, and eigenvectors for the case $\cos \sqrt{\lambda} = 1$ on the left. The respective formulas for these eigenvectors are given by Corollary 3.25 and Corollary 3.27. As before we confined the plots to $k = 0$ and $k = 1$ since a greater k only leads to more edgewise oscillations with similar situations at the edges.

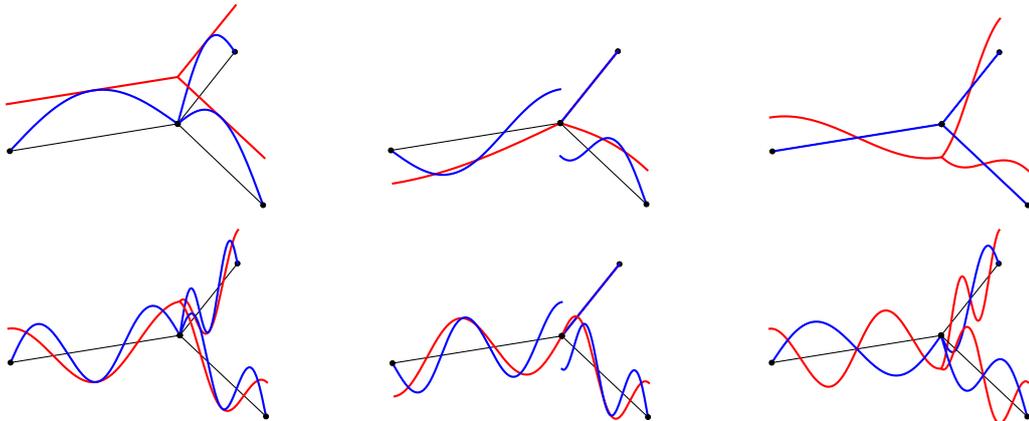


Figure 7: The S_3 eigenfunctions $U_{1,0}$ (top-left), $U_{2,0}$ (top-middle) and $U_{4,0}$ (top-right), as well as $U_{1,1}$ (bottom-left), $U_{2,1}$ (bottom-middle) and $U_{4,1}$ (bottom-right) for the CK case (red) and the KC case (blue), see Corollary 3.25 and Corollary 3.27.

Neither bipartite nor unicyclic The last graph in Table 1 lacks both properties, that we consider here. It is neither bipartite nor unicyclic. Since it has four vertices and five edges ($n = 4, N = 5$) we will refer to this graph as $\Gamma_{4,5}$. As in our second example, the lack of bipartiteness has the consequence, that we cannot apply Corollary 3.36, which would allow us a general comparison between the Kirchhoff and the Anti-Kirchhoff spectrum.

Before we take a closer look at these spectra, we will give the adjacency matrix \mathcal{A} (according to the labeling presented in Figure 4), the transition matrix \mathcal{Z} and the eigenvalues and eigenvectors of \mathcal{Z} , as we did it for the examples above.

$$\mathcal{A} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \quad \mathcal{Z} = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}.$$

$$\sigma(\mathcal{Z}) = \left\{ 1, 0, -\frac{1}{3}, -\frac{2}{3} \right\} \quad \Sigma(\mathcal{Z}) = \begin{pmatrix} 1 & -1 & 0 & -1 \\ 1 & 0 & -1 & \frac{2}{3} \\ 1 & 1 & 0 & -1 \\ 1 & 0 & 1 & \frac{2}{3} \end{pmatrix}$$

Using Corollary 3.24 and 3.26 we obtain the spectra summarized in Table 5. This time there are obviously bigger differences than in the examples before. This holds for the eigenvalues themselves as also for their multiplicities. The differences in the eigenvalues are caused by the lack of bipartiteness, which results in an asymmetric spectrum of the transition matrix \mathcal{Z} . The different multiplicities on the other hand are a consequence of $\Gamma_{4,5}$ not being unicyclic.

	Kirchhoff (CK)	Anti-Kirchhoff (KC)
$\lambda = 0$	$\{0\}$	$\{0\}$
$\cos \sqrt{\lambda} > 0 = 1$	$\{(2k)^2\pi^2 : k \in \mathbb{N}^{(3)}\}$	$\{(2k)^2\pi^2 : k \in \mathbb{N}\}$
$\sin \sqrt{\lambda} \neq 0$	$\{(2k\pi \pm \frac{\pi}{2})^2 : k \in \mathbb{N}_0\} \cup$ $\{(2k\pi \pm \arccos(-\frac{1}{3}))^2 : k \in \mathbb{N}_0\} \cup$ $\{(2k\pi \pm \arccos(-\frac{2}{3}))^2 : k \in \mathbb{N}_0\}$	$\{(2k\pi \pm \frac{\pi}{2})^2 : k \in \mathbb{N}_0\} \cup$ $\{(2k\pi \pm \arccos(\frac{1}{3}))^2 : k \in \mathbb{N}_0\} \cup$ $\{(2k\pi \pm \arccos(\frac{2}{3}))^2 : k \in \mathbb{N}_0\}$
$\cos \sqrt{\lambda} = -1$	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0\}$	$\{(2k+1)^2\pi^2 : k \in \mathbb{N}_0^{(3)}\}$

Table 5: Comparison of the eigenvalues for $\Gamma_{4,5}$

For the ordered spectra, we want to introduce the abbreviations $\alpha_{CK} := \arccos(-1/3)$ and $\beta_{CK} := \arccos(-2/3)$ for the Kirchhoff case. For the Anti-Kirchhoff case we consequently use $\alpha_{KC} := \arccos(1/3)$ and $\beta_{KC} := \arccos(2/3)$. Taking into account the multiplicities of the eigenvalues we obtain the following ordered spectra.

$$\sigma(-\Delta_{\Gamma}^{CK}) = \left\{ 0, \left(\frac{\pi}{2}\right)^2, \alpha_{CK}^2, \beta_{CK}^2, \pi^2, (2\pi)^2, (2\pi)^2, (2\pi)^2, \dots \right\}$$

$$\sigma(-\Delta_{\Gamma}^{KC}) = \left\{ 0, \left(\frac{\pi}{2}\right)^2, \alpha_{KC}^2, \beta_{KC}^2, \pi^2, \pi^2, \pi^2, (2\pi)^2, \dots \right\}$$

Since $\alpha_{KC} < \alpha_{CK}$ and $\beta_{KC} < \beta_{CK}$ we see, that also in this case we cannot find a general inequality for the eigenvalues like $\lambda_j^{CK} \leq \lambda_j^{KC}$ or $\lambda_j^{KC} \leq \lambda_j^{CK}$.

The global scattering matrices in this example can be derived using the local scattering matrices from (35), (36), (37) and (38). The result is presented below in (51). As the determinant of 10×10 matrices the computation of the secular equations is starting to become rather elaborate. An evaluation with a computer-algebra system resulted in a longer expression as in the examples before, which is triggered by the eigenvalues $\alpha_{CK}, \alpha_{KC}, \beta_{CK}$ and β_{KC} that cannot be expressed

as $\frac{p}{q}\pi$, $p, q \in \mathbb{Z}, q \neq 0$. We will therefore not present it here. However, a numerical evaluation of the secular equations at the eigenvalues from Table 5 shows that these values are roots indeed.

The eigenvectors for some of the eigenvalues for both quantum graphs are plotted in Figure 8. A similar selection like in the examples before has been chosen. For the specific formulas of the eigenvectors we again refer to Corollary 3.25 and 3.27.

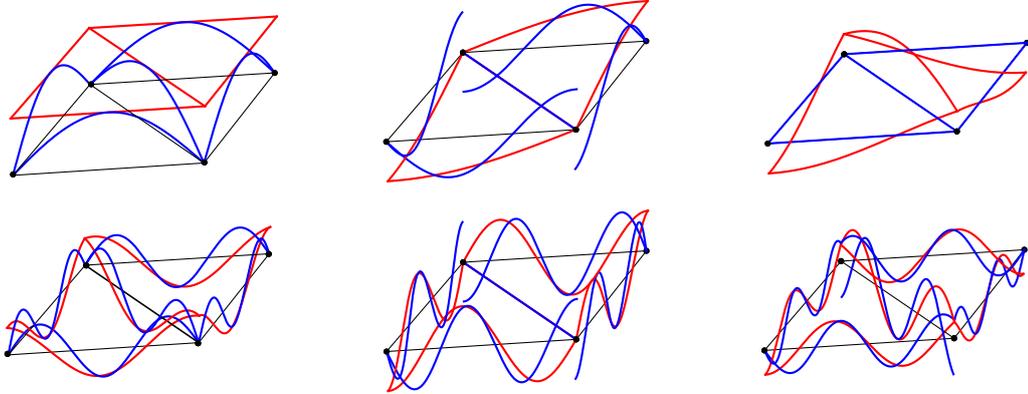


Figure 8: The S_3 eigenfunctions $U_{1,0}$ (top-left), $U_{2,0}$ (top-middle) and $U_{4,0}$ (top-right), as well as $U_{1,1}$ (bottom-left), $U_{2,1}$ (bottom-middle) and $U_{4,1}$ (bottom-right) for the CK case (red) and the KC case (blue), see Corollary 3.25 and Corollary 3.27.

$$S_{CK} = -S_{KC} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 & \frac{2}{3} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & \frac{2}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -\frac{1}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & \frac{2}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & -\frac{1}{3} \\ \frac{2}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 & 0 & -\frac{1}{3} & 0 & 0 \end{pmatrix} \quad (51)$$

4 Conclusion

The spectra of the standard Laplacian on finite equilateral metric graphs under two kinds of vertex conditions, Kirchhoff and Anti-Kirchhoff conditions, have been analyzed, computed and compared with each other. It turned out that both types of vertex conditions result in self-adjoint realizations of the standard Laplacian on compact metric graphs, which have compact resolvent. This result showed that both operators have a discrete spectrum within the nonnegative real numbers. After this qualitative spectral analysis, which showed no difference of the spectra in this regard, a quantitative analysis was performed. During this quantitative approach, using the so-called adjacency calculus introduced by von Below, the specific characteristics of the underlying graph structure were taken into account, and allowed a specific computation of the spectra both for the Kirchhoff and the Anti-Kirchhoff case. The obtained results revealed a spectral relationship in the bipartite case, that can be expressed as an inequality of the ordered spectral elements, depending on the number of cycles within the graph.

The focus of this work was set on equilateral graphs. The effects of variations in the lengths of the edges were not considered. The next step in the comparison of Kirchhoff and Anti-Kirchhoff spectra would therefore be an analysis of compact graphs without the restriction of being equilateral. Von Below already considered this more general case in his dissertation [vB84]. However, his final result was a transcendental characteristic equation, satisfied by the spectral elements, which in most cases can only be solved numerically. It is unclear if this result allows for a general comparison of the spectra as it is possible in the equilateral case.

Appendices

A Functional analysis and Sobolev spaces

The discussion of quantum graph spectra requires numerous results from operator analysis, especially functional analysis. Several classic results we use in the main text are given below with respective sources to read up on the proofs.

Since the theory of differential operators is closely related to Sobolev spaces, we also included some important results from the theory of Sobolev spaces.

A.1 Functional analysis

An elementary but frequently used theorem is the Cauchy-Schwarz inequality, see for example [AU10, Theorem 4.4].

Proposition A.1 (Cauchy-Schwarz inequality). *Let $(U, \langle \cdot, \cdot \rangle)$ be a unitary space with induced norm $\|f\| := \sqrt{\langle f, f \rangle}$. Let $f, g \in U$, then*

$$|\langle f, g \rangle| \leq \|f\| \|g\|$$

Another important result in the context of sesquilinear forms is the polarization identity. It allows us to recover the sesquilinear form from its quadratic form, cf. [Tes, p. 25].

Proposition A.2 (Polarization identity). *Let V be a complex vector space, and $s : V \times V \rightarrow \mathbb{C}$ a sesquilinear form with the associated quadratic form $q(x) = s(x, x)$ then*

$$s(x, y) = \frac{1}{4} \sum_{k=0}^3 i^k q(x + i^k y).$$

Considering linear forms on a Hilbert space, we mention the central representation theorem of Riesz and Fréchet, see [AU10, Theorem 4.21].

Theorem A.3 (Riesz-Fréchet). *Let $\varphi : H \rightarrow \mathbb{C}$ be a continuous linear form on the Hilbert space H . Then there exists a unique $u \in H$ such that φ can be expressed as $\varphi(v) = \langle u, v \rangle$ for all $v \in H$.*

We turn our attention to spectral theory. When we consider bounded or even compact operators we can characterize their spectra using the following two classic results. We refer to [Mug17, Theorem 7.1.10, 7.1.13] and [Mug17, Theorem 7.7.1, 7.7.3].

Proposition A.4 (Spectrum of bounded operators). *Let $T \in \mathcal{L}(X)$ with X being a Banach space over the complex numbers \mathbb{C} . Then $\sigma(T)$ is a nonempty and compact subset of \mathbb{C} .*

Proposition A.5 (Spectrum of compact operators). *Let X be a Banach space and $K \in \mathcal{K}(X)$ a compact operator, then its spectrum $\sigma(K)$ can be characterized as follows.*

- (i) $\sigma(K)$ is either a finite or countable infinite set.
- (ii) All $\lambda \in \sigma(K)$ have finite multiplicity.
- (iii) $\lambda \in \sigma(K) \setminus \{0\} \Rightarrow \lambda \in \sigma_p(K)$
- (iv) $\sigma_p(K)$ can only accumulate at 0.
- (v) If $\dim X = \infty$ then $0 \in \sigma(K)$.

In the context of bounded self-adjoint operators we use the following two results regarding their spectrum, cf. [Mug17, Theorem 7.1.23] and [PS99, Theorem 7.9].

Lemma A.6. *Let T be a bounded self-adjoint operator on the Hilbert space H . Then we have*

$$\sup\{|\lambda| : \lambda \in \sigma(T)\} = \|T\|$$

Lemma A.7 (Self-adjoint inverse). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be a self-adjoint invertible operator. Then T^{-1} is self-adjoint too.*

In the context of the resolvent operator we mention the following results. We refer to [Wei12, Theorem 5.13], [Are, Proposition 1.2.2] and [Are, Proposition 1.2.3].

Lemma A.8 (Resolvent identity). *Let T be a closed operator with $\lambda, \mu \in \rho(T)$. Then*

$$R(\lambda, T) - R(\mu, T) = (\mu - \lambda)R(\lambda, T)R(\mu, T).$$

Proposition A.9. (Analyticity of the resolvent) *Let $T : H \supset \text{dom}(T) \rightarrow H$ be an operator, $\lambda_0 \in \rho(T)$ and $\lambda \in \mathbb{C}$ such that $|\lambda - \lambda_0| < \|R(\lambda_0, T)\|^{-1}$. Then it follows $\lambda \in \rho(T)$ and*

$$R(\lambda, T) = \sum_{n=0}^{\infty} (\lambda_0 - \lambda)^n R(\lambda_0, T)^{n+1}.$$

Corollary A.10. *Let $T : H \supset \text{dom}(T) \rightarrow H$ be an operator with nonempty resolvent set, and let $(\lambda_n) \subset \rho(T)$ be a convergent sequence with $\lim \lambda_n = \lambda$. If $\sup_{n \in \mathbb{N}} \|R(\lambda_n, T)\| < \infty$ then $\lambda \in \rho(T)$.*

We conclude this section by stating the spectral theorem. It asserts that any self-adjoint operator can essentially be understood as a multiplication operator. We refer to [Wer11, Definition VII.3.1].

Theorem A.11 (Spectral Theorem). *Let $T : H \supset \text{dom}(T) \rightarrow H$ be a self-adjoint operator. Then there exists a measure space (Ω, Σ, μ) , a measurable function $f : H \rightarrow \mathbb{R}$ and a unitary operator $U : H \rightarrow L^2(\Omega, \Sigma, \mu)$ such that*

- (i) $x \in \text{dom}(T) \Leftrightarrow f \cdot Ux \in L^2(\Omega, \Sigma, \mu)$;
- (ii) $UTU^*\varphi = f \cdot \varphi =: M_f(\varphi)$ for all $\varphi \in \text{dom}(M_f) = \{\varphi \in L^2(\Omega, \Sigma, \mu) : f \cdot \varphi \in L^2(\Omega, \Sigma, \mu)\}$.

A.2 Sobolev and Lebesgue spaces

Our only result specifically for Lebesgue spaces states the density of $C_0^\infty(a, b)$ in $L^p(a, b)$, see for example [Mug17, Theorem 5.1.21].

Proposition A.12. *Let $(a, b) \subset \mathbb{R}$ be an open real interval and $1 \leq p < \infty$, then the space $C_0^\infty(a, b)$ is dense in $L^p(a, b)$.*

The following elementary results for one dimensional Sobolev spaces is taken from [Mug17, Theorem 5.3.28].

Theorem A.13. *Let $I = [a, b] \subset \mathbb{R}$ be a compact real interval, then $H^1(a, b) \subset C(a, b)$.*

We introduce the important notion of an embedding, and refer to [AF03, Definition 1.25].

Definition A.14 (Embedding). *Let X, Y be two normed spaces. We say that X is embedded in Y , which we will denote by $X \hookrightarrow Y$, if X is a subspace of Y and the identity operator defined as $\text{Id} : X \rightarrow Y, x \mapsto x$ is continuous. If the injection Id is even compact we say that X is compactly embedded in Y , which we will denote as $X \overset{c}{\hookrightarrow} Y$.*

There are numerous embeddings that can be stated, depending on different geometric conditions of the domain (which is just a finite interval in our case). They can all be found in [AF03, Theorem 6.3]. For our purposes we only need one of the compact embeddings which is stated below without proof.

Theorem A.15 (Rellich-Kondrachov). *Let $I \subset \mathbb{R}$ be a bounded real interval. Furthermore let $j, m \in \mathbb{N}$ with $j \geq 0$ and $m \geq 1$ and $1 \leq p, q < \infty$. Then*

$$W^{j+m, p}(I) \overset{c}{\hookrightarrow} W^{j, q}(I)$$

B Linear algebra and graph theory

Graph theory and related theorems from linear algebra require several different notions that are given below. While most of the presented material just introduces the required vocabulary, we also state the theorem of Perron-Frobenius, which provides us with information on the spectrum of nonnegative, irreducible matrices.

B.1 Linear algebra

The following three definitions introduce three kinds of special matrices, that we encounter in our graph theoretic considerations.

Definition B.1 (Nonnegative matrix). *We call a matrix $A = (a_{ij}) \in \mathbb{R}^{n \times m}$ of arbitrary shape nonnegative, if $a_{ij} \geq 0$ for all $i \in \{1, \dots, n\}$ and all $j \in \{1, \dots, m\}$.*

Definition B.2 (Irreducible matrix). *Let $A \in \mathbb{R}^{n \times n}$ be a square matrix. We call A reducible if we can find a permutation matrix $P \in \mathbb{R}^{n \times n}$ such that*

$$PAP^T = \begin{pmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{pmatrix}$$

with the block matrices $A_{11} \in \mathbb{R}^{r \times r}$ and $A_{21} \in \mathbb{R}^{(n-r) \times r}$ and $A_{22} \in \mathbb{R}^{(n-r) \times (n-r)}$. If we cannot find such a matrix P we say that A is irreducible.

Definition B.3 (Stochastic matrix). *A square matrix $S = (s_{ij}) \in \mathbb{R}^{n \times n}$ with $0 \leq s_{ij} \leq 1$ for all $1 \leq i, j \leq n$ is said to be row-stochastic if $\sum_{j=1}^n s_{ij} = 1$ for all $i \in \{1, \dots, n\}$. If $\sum_{i=1}^n s_{ij} = 1$ for all $j \in \{1, \dots, n\}$ then we say that S is column-stochastic. If finally S is both row- and column-stochastic, we also say that S is stochastic or doubly-stochastic.*

Row-stochastic matrices have some nice properties regarding their eigenvalues. Since the transition matrix $\mathcal{Z}(\Gamma)$ of a graph Γ is row-stochastic, this result is very useful for us [KB12, p. 907].

Proposition B.4. *Let $S \in \mathbb{R}^{n \times n}$ be a row-stochastic matrix, then $\mu = 1$ is an eigenvalue of S with the eigenvector $e := (1)_{n \times 1}$. Furthermore, if $\lambda \in \sigma(S)$, then $|\lambda| \in [0, 1]$.*

The next result is known as the theorem of Perron-Frobenius. It provides us with information on the spectra for nonnegative and irreducible matrices. We refer to [KB12, Theorem 8.51].

Theorem B.5 (Perron-Frobenius). *Let $A \in \mathbb{R}^{n \times n}$ be an irreducible nonnegative matrix. Then $\lambda = \text{rad}(A)$ is a simple eigenvalue of A corresponding to a positive eigenvector $v \in \mathbb{R}^n$, i.e., $v > 0$.*

It remains to introduce the so-called Hadamard product, which refers to a component-wise matrix multiplication. We state here a formal introduction, alongside with some obvious properties, and refer to [vB85, Section 3].

Definition B.6 (Hadamard product). *Let $A := (a_{ij})_{n \times m} \in \mathbb{C}^{n \times m}$ and $B := (b_{ij})_{n \times m} \in \mathbb{C}^{n \times m}$ be two matrices with identical shapes. We define the so-called Hadamard-product as to*

$$A \cdot B = (a_{ij}b_{ij})_{n \times m}$$

Proposition B.7 (Hadamard product rules). *Let A, B, C be identical shaped matrices as described in Definition B.6. Then the following identities hold.*

$$\begin{aligned} A \cdot B &= B \cdot A \\ (A \cdot B)^* &= A^T \cdot B^* \\ (A + B) \cdot C &= A \cdot C + B \cdot C \end{aligned}$$

B.2 Graph theory

Given some graph $\Gamma = (V, E)$ with two vertices $v_1, v_2 \in V$ with $v_1 \neq v_2$ we can think of walking from v_1 to v_2 in a way, that is described in the following definition.

Definition B.8 (Walk). *Let $\Gamma = (V, E)$ be a graph according to Assumption 2.32. A finite sequence of edges $(e_{i_1}, e_{i_2}, \dots, e_{i_k})$ with $e_{i_j} \cap e_{i_{j+1}} \neq \emptyset$ is called a walk.*

The term of a walk is rather general, since edges may occur several times. If we do not allow the multiple use of edges in a walk, we end up at the definition of a trail.

Definition B.9 (Trail). *Let $\Gamma = (V, E)$ be a graph according to Assumption 2.32. A walk $(e_{i_1}, e_{i_2}, \dots, e_{i_k})$ with distinct edges is called a trail.*

Since we now ensured that the edges in a trail occur at most one time, we can analogously require that the vertices of the edges are not reused, i.e., that the trail does not intersect itself. This brings us to the notion of the path.

Definition B.10 (Path). *Let $\Gamma = (V, E)$ be a graph according to Assumption 2.32. Also, let $p := (e_{i_1}, e_{i_2}, \dots, e_{i_k})$ be a trail of the graph with $\Gamma_p = (V_p, E_p)$ being the graph of the trail. If $\gamma_v \leq 2$ for all $v \in V_p$ with respect to Γ_p then we call p a path.*

All vertices on a path are lying on exactly two edges of the path, with the only possible exceptions being the first and the last node, each of which may only lie on one edge of the path. If this is not the case, then the first and the last vertex have to be identical. Such a structure we call a cycle.

Definition B.11 (Cycle). *Let $\Gamma = (V, E)$ be a graph according to Assumption 2.32. Also, let $p := (e_{i_1}, e_{i_2}, \dots, e_{i_k})$ be a path of the graph with $\Gamma_p = (V_p, E_p)$ being the graph of the path. If the first and the last node coincide, i.e., $\gamma_v = 2$ for all $v \in V_p$ with respect to Γ_p then we call p a cycle.*

Not all graphs need to contain a cycle. With this observation we can define our first special kind of graph, i.e., graphs that do not contain a cycle. For this group there exists a specific name.

Definition B.12 (Tree graph). *A graph $\Gamma = (V, E)$ corresponding to Assumption 2.32 is said to be a tree or a tree graph if it contains no cycles.*

A cycle is also often called a circuit in the literature. We will use the term cycle though because it is consistent with our next definition, which is the second special type of graph we introduce here.

Definition B.13 (Unicyclic graph). *A graph $\Gamma = (V, E)$ corresponding to Assumption 2.32 is said to be unicyclic, if there exists a cycle c in Γ , and all other cycles contain the same edges as c .*

Unicyclic graphs contain exactly one cycle, if we do not distinguish cycles with different numberings of the edges. An important property of unicyclic graphs is given by the following lemma.

Lemma B.14. *Let $\Gamma = (V, E)$ be a given graph that is satisfying Assumption 2.32. Then Γ is unicyclic if and only if its number of edges and vertices coincide, i.e., $|V| = |E|$.*

Unicyclic graphs can hence be characterized as the set of graphs whose numbers of vertices and edges coincide. Another special group of graphs are the so-called bipartite graphs.

Definition B.15 (Bipartite graph). *Let $\Gamma = (V, E)$ be a given graph that is satisfying Assumption 2.32. If we can find disjoint $V_1, V_2 \subset V$ with $V_1 \cup V_2 = V$ such that $e \cap V_1 \neq \emptyset$ and $e \cap V_2 \neq \emptyset$ for all $e \in E$ we say that Γ is bipartite.*

The vertex set of a bipartite graph can be split into two disjoint sets, such that every edge of the graph contains one vertex of each of these sets. We can also express this situation by saying that each of the disjoint vertex sets is not interconnected.

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Ich erkläre, dass ich die vorliegende Abschlussarbeit mit dem Thema *Spectral comparison of the standard Laplacian on equilateral finite metric graphs subjected to Kirchhoff and Anti-Kirchhoff vertex conditions* selbstständig und ohne unzulässige Inanspruchnahme Dritter verfasst habe. Ich habe dabei nur die angegebenen Quellen und Hilfsmittel verwendet und die aus diesen wörtlich, inhaltlich oder sinngemäß entnommenen Stellen als solche den wissenschaftlichen Anforderungen entsprechend kenntlich gemacht. Die Versicherung selbstständiger Arbeit gilt auch für Zeichnungen, Skizzen oder graphische Darstellungen. Die Arbeit wurde bisher in gleicher oder ähnlicher Form weder derselben noch einer anderen Prüfungsbehörde vorgelegt und auch noch nicht veröffentlicht. Mit der Abgabe der elektronischen Fassung der endgültigen Version der Arbeit nehme ich zur Kenntnis, dass diese mit Hilfe eines Plagiatserkennungsdienstes auf enthaltene Plagiate überprüft und ausschließlich für Prüfungszwecke gespeichert wird. Außerdem räume ich dem Lehrgebiet das Recht ein, die Arbeit für eigene Lehr- und Forschungstätigkeiten auszuwerten und unter Angabe des Autors geeignet zu publizieren.

Hagen, den (Abgabedatum)

Mark Alexander Klawonn