Spectral Theory of Differential Operators on Finite Metric Graphs and on Bounded Domains

Dissertation zur Erlangung des Grades

Doktor der Naturwissenschaften

am Fachbereich Physik, Mathematik und Informatik
der Johannes Gutenberg–Universität Mainz

vorgelegt
von

Amru Hussein
geboren in Hannover

Mainz im Januar 2013

Dekan:

Erster Gutachter:

Zweiter Gutachter:

Tag der Promotion: 18. Juli 2013

لِذِكْرَةِ ٱلْمَرْحُومَةِ
ٱلْدَكْتُورَةِ

خَضْرَة قَبْلَاوِي

In memory of

Khadra Kablawie

اَلْعِلْمُ نُوْر

Zusammenfassung

Die vorliegende Arbeit widmet sich der Spektraltheorie von Differentialoperatoren auf metrischen Graphen und von indefiniten Differentialoperatoren auf beschränkten Gebieten. Sie besteht aus zwei Teilen. Im Ersten werden endliche, nicht notwendigerweise kompakte, metrische Graphen und die Hilberträume von quadratintegrierbaren Funktionen auf diesen betrachtet. Alle quasi–m–akkretiven Laplaceoperatoren auf solchen Graphen werden charakterisiert, und Abschätzungen an die negativen Eigenwerte selbstadjungierter Laplaceoperatoren werden hergeleitet.

Weiterhin wird die Wohlgestelltheit eines gemischten Diffusions- und Transportproblems auf kompakten Graphen durch die Anwendung von Halbgruppenmethoden untersucht.

Eine Verallgemeinerung des indefiniten Operators $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ von Intervallen auf metrische Graphen wird eingeführt. Die Spektral- und Streutheorie der selbstadjungierten Realisierungen wird detailliert besprochen.

Im zweiten Teil der Arbeit werden Operatoren untersucht, die mit indefiniten Formen der Art $\langle \operatorname{grad} v, A(\cdot) \operatorname{grad} u\rangle$ mit $u, v \in H^1_0(\Omega) \subset L^2(\Omega)$ und $\Omega \subset \mathbb{R}^d$ beschränkt, assoziiert sind. Das Eigenwertverhalten entspricht in Dimension $d = 1$ einer verallgemeinerten Weylschen Asymptotik und für $d \geq 2$ werden Abschätzungen an die Eigenwerte bewiesen. Die Frage, wann indefinite Formmethoden für Dimensionen $d \geq 2$ anwendbar sind, bleibt offen und wird diskutiert.

Abstract

This thesis is devoted to the spectral theory of differential operators on metric graphs and of indefinite differential operators on bounded domains. It consists of two parts. In the first part finite not necessarily compact metric graphs and the Hilbert spaces of square integrable functions on these graphs are considered. All quasi–m–accretive Laplacians on such graphs are characterized and estimates on the negative eigenvalues of self–adjoint Laplacians are derived.

Furthermore the well-posedness of a mixed transport and diffusion problem on a compact metric graph is studied in terms of semigroups.

The indefinite operator $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ is generalized from intervals to finite metric graphs. The spectral and the scattering theory of the self–adjoint realizations are elaborated in detail.

In the second part operators are studied that are associated with indefinite quadratic forms of the type $\langle \operatorname{grad} v, A(\cdot)\operatorname{grad} u\rangle$, where $u, v \in H_0^1(\Omega) \subset L^2(\Omega)$ and $\Omega \subset \mathbb{R}^d$ bounded. In dimension $d = 1$ the asymptotic distribution of eigenvalues satisfies a generalized Weyl law and for dimension $d \geq 2$ estimates on the eigenvalues are derived. The problem when indefinite form methods apply in dimensions $d \geq 2$ constitutes an open problem and is discussed as well.

Contents

Introduction

Spectral theory provides a connection between differential equations and functional analysis. The fast developments in natural science and engineering have made linear differential operators on metric graphs as well as sign–indefinite second order differential operators on bounded domains subjects of practical and scientific relevance. Both are the main topics of this thesis.

Differential equations and, consequently, differential operators on metric graphs arise from models for systems on quasi–one–dimensional structures. Quasi–one–dimensional means that these structures have very small extension in all but the longitudinal direction. Such structures appear in many models of mesoscopic physics and nanotechnology like carbon nano tubes, thin quantum wires or photonic crystals, but also in many other fields of science, see [60, 71] and the references therein. One can model these structures mathematically by domains or manifolds which are bordered by a thin neighbourhood of a certain metric graph. Such a thin neighbourhood of a graph is sometimes called "thick graph". For many classical questions of physics, such as heat conduction or the quantum mechanical description of an electron, there are well–developed theories. However, in many concrete situations a direct analytic approach is not feasible since the data are too extensive and one has to rely on numerical methods for obtaining at least approximate solutions. An alternative is to reduce the model until one arrives at an explicitly solvable setting. Such solvable models can be used for qualitative analysis and for refining the understanding of the original situation. For quasi–one–dimensional structures one simplification consists in restricting the model only to the graph. For example, the state of an electron in a quantum wire can also be described by the one–dimensional Schrödinger equation which furnishes a solvable model for this situation.

The relation between certain operators on "thick graphs" and those on the corresponding metric graphs is considered in many research works, see for example [36,41]. The application of graph models in science and engineering has a long history and its popularity is still increasing, see for example [60, 71] and the references cited therein. The focus of this thesis lies on the mathematical analysis of various solvable models on metric graphs.

A metric graph can roughly be thought of as a finite union of intervals glued together at their end points. Differential operators are considered on each edge separately and are coupled using boundary conditions. In particular, the study of self–adjoint Laplace operators on metric graphs has become famous under the name "quantum graphs", see for example [14, 72] and the references therein. The present work ties in with this subject. However, the work does not remain in the framework of this well developed theory, but it carries over the corresponding techniques to develop new models on graphs, in particular models involving different types of dynamics simultaneously.

Indefinite differential operators of the form $-\operatorname{div} A(\cdot) \operatorname{grad}$ appear in different contexts. The Poisson problem related to the corresponding operator is of physical relevance, since it appears in the description of light propagation through regions filled by materials with negative and positive refraction indices. Materials with negative refraction index have become famous under the name metamaterials and they exhibit specific unusual refraction properties, see [22] and the references therein. Another field of application is solid state–physics. In the effective mass approximation, the effective mass of a particle is a tensor which can also have changing sign, see for example [3, 100] and the references therein.

This thesis consists of two parts. The first part is devoted to the study of linear differential operators on metric graphs, primarily to their spectral properties, whereas the second part deals with the spectral theory of certain linear indefinite second order differential operators on bounded domains with Dirichlet boundary conditions. Each chapter of Part 1 deals with a specific question and each can be considered basically on its own. The content of the Chapters 1, 2, 3 and 4 has been published in parts as preprints, see [51], [53], [54] and [52], respectively.

The first chapter gives a characterization of all boundary conditions yielding quasi–m–accretive Laplacians on finite metric graphs. An operator is quasi–m–accretive if its numerical range as well as the numerical range of its adjoint is contained in a certain right half–plane of the complex plane. A particular case of such operators are self–adjoint Laplace operators which are semi–bounded from below. In the context of quantum mechanics self–adjointness of Hamiltonians corresponds to the conservative character of the system. However, there are further applications, particularly stochastic processes on graphs, which do not require self–adjointness. For the study of the diffusion equation with initial conditions, it is enough to require that the solution to this problem is governed by certain one–parameter semigroups. Now, the infinitesimal generators of quasi–contractive semigroups are exactly minus the quasi–m–accretive operators. Therefore, characterizing these operators solves the problem of the well–posedness of the initial value problem for the diffusion equation on metric graphs. From this one additionally obtains an explicit characterization of all boundary conditions defining m–accretive Laplacians on finite metric graphs. These are the infinitesimal generators of contractive semigroups. This improves the results of V. Kostrykin and R. Schrader on m–accretive Laplace operators on finite metric graphs, see [64].

The growth bound of a quasi–contractive semigroup provides information on the stability of the system and it is related to the negative spectrum of a certain self–adjoint Laplace operator on the graph. This motivates the study of the negative eigenvalues of self–adjoint Laplacians on finite metric graphs in Chapter 2. Upper and lower bounds on each of the negative eigenvalues of such operators are derived, and the question of optimality of the resulting lower bounds on the spectrum is discussed. In particular, one obtains a priori estimates from below and from above on the growth bound of the corresponding semigroup, and in addition the formerly known lower bounds on the spectrum derived by P. Kuchment, see [72], and V. Kostrykin and R. Schrader, see [63], are re–obtained. These previously known bounds are depending only on the smallest edge length of the graph, whereas some of the estimates derived here involve all edges. The proofs use variational methods for certain non–linear operator pencils.

Chapter 3 deals with mixed parabolic–hyperbolic dynamics on compact metric graphs. This is motivated by a neuron model, where transport features are used to model time delays at vertices. The simultaneous consideration of dynamics of different types is a new aspect in the theory of differential operators on metric graphs. Here, a system is described which on some edges is given by the transport equation and on some edges by the diffusion equation. Picking up the thread of the theories of transport and diffusion on metric graphs, which so far have been studied separately, I consider the first and the second order derivative operator and implement couplings by means of boundary conditions. These boundary conditions define quasi–m–dissipative operators which, in turn, generate quasi–contractive semigroups describing a mixed transport and diffusion evolution on the graph. Several properties of these semigroups can be described by means of the spectral theory of their infinitesimal generators. This chapter is based on joint work with Delio Mugnolo, see [54].

Chapter 4 deals with an operator that is defined on each edge either by "plus Laplace" or by "minus Laplace". This is a straightforward generalization of the operator $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ to metric graphs. This can be interpreted as a case of mixed dynamics, where one has to match "plus Laplace" and "minus Laplace" to a self–adjoint operator and it is a simplified model for the problem discussed in Part 2. All self–adjoint realizations of these differential expressions are characterized in terms of explicit parametrizations. The spectral along with the scattering theory for these operators is discussed in detail. This model problem exhibits many new and unusual features, especially the scattering properties. Applying an approach that uses generalizations of the first representation theorem to unbounded and indefinite quadratic forms yields natural boundary conditions on each vertex, which are related to the standard or Kirchhoff boundary conditions for Laplace operators on metric graphs. This model problem for a sign–indefinite second order differential operator builds a bridge to the subject of Part 2.

As already mentioned, the second part is devoted to the construction and study of self–adjoint differential operators formally given by the expression $\mathcal{L} = -\operatorname{div} A(\cdot)\operatorname{grad}$. The main concern is the spectrum of such operators.

Recall that for $A(\cdot)$ strongly elliptic and sufficiently regular the classical representation theorems apply, and hence there is a unique semi–bounded self–adjoint operator which is associated with the form defined by $\langle \operatorname{grad} u, A(\cdot)\operatorname{grad} v\rangle$ in the Hilbert space $L^2(\Omega)$. Dropping the assumption that the function $A(\cdot)$ has a constant sign, the questions of symmetric forms and self–adjoint operators associated with them becomes more delicate. The notion of closedness of a form is essential for the formulation and the proofs of the classical representation theorems, but this notion is defined only for semi–bounded forms, and if $A(\cdot)$ has non–constant sign then the form given by $\langle \operatorname{grad} u, A(\cdot)\operatorname{grad} v\rangle$ is evidently not semi–bounded.

However, there is a generalization of closedness to non–semi–bounded symmetric forms which is due to A. G. R. McIntosh, see [75], and in addition there are also generalizations of the classical representation theorems for symmetric semi–bounded forms to non–semi–bounded symmetric forms. Later, also a Krein space approach has been used to deal with sign–indefinite forms, see [38], and recently the above mentioned results have been collected and new simplified proofs have been provided for the generalizations of the representation theorems, see [43], where also an overview and a brief history of this topic can be found.

In Chapter 5, this theory is applied to the problem of sign–indefinite differential operators of the form $\mathcal{L} = -\operatorname{div} A(\cdot)\operatorname{grad}$ on bounded Lipschitz domains with Dirichlet boundary conditions. It is required that such an operator is associated with the possibly indefinite symmetric unbounded form $\mathfrak{l}$ defined by $\mathfrak{l}[u,v] = \langle \operatorname{grad} u, A(\cdot)\operatorname{grad} v\rangle$ with domain $H^1_0(\Omega) \subset L^2(\Omega)$. In certain situations the operator $\mathcal{L}$ can be constructed from the form $\mathfrak{l}$ by applying a generalization of the first representation theorem. This approach involves the assumption that the form given by $\mathfrak{l}[u,v]$ now considered as a form in the Hilbert space $H^1_0(\Omega)$, determines a bounded and boundedly invertible operator. In the terminology of A. G. R. McIntosh such forms are called

0–closed, see [75, Section 3]. In fact, if $\mathfrak{l}$ is 0–closed, there is unique self–adjoint operator $\mathcal{L}$ associated with this form and the spectrum of $\mathcal{L}$ is purely discrete.

Chapter 6 deals with the asymptotic distribution of the eigenvalues of the sign–indefinite operator $\mathcal{L}$. In dimension $d = 1$, the spectrum of the operator $\mathcal{L}$ constructed in Chapter 5 asymptotically resembles the spectrum of the sum of a positive definite and a negative definite operator. This is reflected by the asymptotic behaviour of the eigenvalues of $\mathcal{L}$ which satisfy a generalized Weyl law. This motivates a general conjecture on the asymptotic behaviour of the eigenvalue counting functions of $\mathcal{L}$. For dimension $d \geq 2$, bounds on the eigenvalue counting functions are derived, and in specific situations the conjectured distribution forms a lower bound on the eigenvalue counting functions. The proofs are based on variational arguments, which are applied to the unbounded and indefinite operator $\mathcal{L}$. This permits to compare the eigenvalue problem for $\mathcal{L}$ to certain generalized eigenvalue problems.

For dimensions greater than one, there is no general criterion available at present to check for given $A(\cdot)$ whether the form $\mathfrak{l}$ is 0–closed. It is therefore an open problem in which situations the theory presented here can be applied. Examples where the form $\mathfrak{l}$ is 0–closed and where $\mathfrak{l}$ is not 0–closed are discussed in Chapter 5 in detail. Nevertheless, new aspects in the still developing theory of indefinite second order differential operators on bounded domains are discovered. From the pedagogical point of view the study provides a good understanding of the form approach for closed semi–bounded forms. Part 2 is based on a ongoing joint work with Vadim Kostrykin, David Krejčiřík and Stephan Schmitz, [56].

Acknowledgements. First of all I would like to thank V. K. for getting involved in my PhD project as supervisor for my thesis and engaging with me in helpful discussions and raising valuable questions. Furthermore I am grateful to him for pointing out many references. In particular for the content of the Chapters 1 and 2 the references [89] and [12] have been essential. I am grateful to A. L. for making the last mentioned work accessible for me prior to publication. I am also thankful to P. S. for communicating and discussing Example 1.11 in Chapter 1 and to T. S. for pointing out the article [17] to the functional analysis group at the university of Mainz which I am part of. Also, I would like to thank very much P. E. for acting as second referee for this thesis.

I am grateful to D. K. for communicating the problems related to sign–indefinite second order differential operators and their physical background, for helpful discussions as well as for his remarks and advice. Especially I want to thank him for the kind hospitality during my visit to the Doppler Institute in Prague in February 2012.

I thank D. M. for getting in touch with me to initiate the collaboration on the problem elaborated in [54], which is presented here partially in Chapter 3. Furthermore true thanks to him for his hospitality during my visit to the research group "Symmetriemethoden in Quantengraphen" in Ulm in January 2012.

For many discussions, constant support and encouragement I thank S. L. I am also very grateful to my colleagues M. H., A. S. and S. Sch., with whom I spend the years of my doctorate, not only for a great deal of discussion, but also for chats and coffee. They also read parts of this thesis and gave me useful suggestions. I thank very much S. L.–G. for the careful reading of the manuscript. Furthermore I thank H.–P. H., St. F., C. K. and E. P. M. for valuable support.

This thesis is in memory of my late mother. We grew up with the development of her dissertation, [55], and without her appreciation for education and learning I would not have taken this path.

Part 1

Differential operators on finite metric graphs

Basic concepts

Finite metric graphs. The basic concept of this part is the one of metric graphs. A metric graph is a locally linear one dimensional space with singularities at the vertices. One can think roughly of a metric graph as a finite union of intervals $[0, a_i]$, $a_i > 0$ or $[0, \infty)$ glued together at their end points. The notation and basic definitions are borrowed from the works of V. Kostrykin and R. Schrader, compare for example [60, 62, 63]. They are summarized here briefly and are complemented with some additional features which are needed for the more general purpose of this work. On these lines a *graph* is the 4-tuple

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

where V denotes the set of *vertices*, $\mathcal{I}$ the set of *internal edges* and $\mathcal{E}$ the set of *external edges*. The set $\mathcal{E} \cup \mathcal{I}$ is summed up in the notion *edges*. The *boundary map* ∂ assigns to each internal edge $i \in \mathcal{I}$ an ordered pair of vertices $\partial(i) = (v_1, v_2) \in V \times V$, where $\partial^-(i) := v_1$ is called its *initial vertex* and $\partial^+(i) := v_2$ its *terminal vertex*. Each external edge $e \in \mathcal{E}$ is mapped by ∂ to a single, its initial vertex $\partial(e) \in V$. In particular the above definition allows a graph to have loops and multiple edges.

The *degree* $\deg(v)$ of a vertex $v \in V$ is the number of edges with initial vertex v plus the number of edges with terminal vertex v. A graph is called *finite* if $|V| + |\mathcal{I}| + |\mathcal{E}| < \infty$ and a finite graph is called *compact* if $\mathcal{E} = \emptyset$.

The graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ can be endowed with a metric structure. Each internal edge $i \in \mathcal{I}$ is identified with an interval $[0, a_i]$ with $a_i > 0$, such that its initial vertex $\partial^-(i)$ corresponds to 0 and its terminal vertex $\partial^+(i)$ to a_i. Each external edge $e \in \mathcal{E}$ is identified with the half line $[0, \infty)$, such that $\partial(e)$ corresponds to 0. The numbers a_i are called *lengths* of the internal edges $i \in \mathcal{I}$, and they are summed up into the vector

$$\underline{a} = \{a_i\}_{i \in \mathcal{I}} \in \mathbb{R}_+^{|\mathcal{I}|}.$$

The 2-tuple $(\mathcal{G}, \underline{a})$ consisting of the finite graph $\mathcal{G}$, which is endowed with the metric structure induced by $\underline{a}$ is called *metric graph*. The metric on $(\mathcal{G}, \underline{a})$ is defined via minimal path lengths on it. This makes out of $(\mathcal{G}, \underline{a})$ a metric space and together with the Lebesgue measure on each edge a measure space.

Any function $\psi\colon (\mathcal{G}, \underline{a}) \to \mathbb{C}$ can be written as

$$\psi(x_j) = \psi_j(x), \quad \text{where} \quad \psi_j\colon I_j \to \mathbb{C}$$

with

$$I_j = \begin{cases} [0, a_j], & \text{if } j \in \mathcal{I}, \\ [0, \infty), & \text{if } j \in \mathcal{E}. \end{cases} \tag{1}$$

One defines

$$\int_{\mathcal{G}} \psi := \sum_{i\in\mathcal{I}} \int_0^{a_i} \psi(x_i)\, dx_i + \sum_{e\in\mathcal{E}} \int_0^{\infty} \psi(x_e)\, dx_e, \tag{2}$$

where dx_i and dx_e refers to integration with respect to the Lebesgue measure on the intervals $[0, a_i]$ and $[0, \infty)$, respectively.

Matrix valued functions are going to be used frequently in the context of metric graphs $(\mathcal{G}, \underline{a})$. For a function f one denotes by $f(\underline{a})$ the $|\mathcal{I}| \times |\mathcal{I}|$–diagonal matrix with entries

$$\{f(\underline{a})\}_{i,j\in\mathcal{I}} = \delta_{ij} f(a_i), \tag{3}$$

where δ_{ij} is the Kronecker delta.

Function spaces. Given a finite metric graph $(\mathcal{G}, \underline{a})$ one considers the Hilbert space

$$\mathcal{H} \equiv \mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}_{\mathcal{E}} \oplus \mathcal{H}_{\mathcal{I}}, \quad \mathcal{H}_{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \mathcal{H}_e, \quad \mathcal{H}_{\mathcal{I}} = \bigoplus_{i\in\mathcal{I}} \mathcal{H}_i, \tag{4}$$

where $\mathcal{H}_j = L^2(I_j; \mathbb{C})$ with I_j as in (1). The scalar product in the Hilbert space $\mathcal{H}$ is denoted by $\langle\cdot,\cdot\rangle = \langle\cdot,\cdot\rangle_{\mathcal{H}}$ and the induced norm by $\|\cdot\| = \|\cdot\|_{\mathcal{H}}$.

In this part of the thesis ordinary differential operators of order one or two defined on each edge are considered within the framework of Hilbert space theory. To provide suitable domains of definition for operators and forms appropriate Sobolev spaces are introduced. By $\mathcal{W}_j$ with $j \in \mathcal{E} \cup \mathcal{I}$ one denotes the set of all $\psi_j \in \mathcal{H}_j$ such that ψ_j is absolutely continuous and it derivative ψ_j' is square integrable. Let $\mathcal{W}_j^0$ denote the set of all those elements $\psi_j \in \mathcal{W}_j$ with

$$\begin{aligned} &\psi_j(0) = 0, \quad \text{for} \quad j \in \mathcal{E},\\ &\psi_j(0) = 0 \quad \text{and} \quad \psi_j(a_j) = 0, \text{ for } j \in \mathcal{I}. \end{aligned}$$

On the whole metric graph one considers the direct sums of these spaces

$$\mathcal{W} \equiv \mathcal{W}(\mathcal{E}, \mathcal{I}) = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{W}_j, \quad \text{and} \quad \mathcal{W}^0 \equiv \mathcal{W}^0(\mathcal{E}, \mathcal{I}) = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{W}_j^0. \tag{5}$$

Denote by $\mathcal{D}_j$ with $j \in \mathcal{E} \cup \mathcal{I}$ the set of all $\psi_j \in \mathcal{H}_j$ such that ψ_j and its derivative ψ_j' are absolutely continuous and its second derivative ψ_j'' is square integrable. Let $\mathcal{D}_j^0$ denote the set of all those elements $\psi_j \in \mathcal{D}_j$ with

$$\begin{aligned} &\psi_j(0) = 0, \quad \psi_j'(0) = 0, \quad \text{for } j \in \mathcal{E},\\ &\psi_j(0) = 0, \quad \psi_j'(0) = 0, \quad \psi_j(a_j) = 0, \ \psi_j'(a_j) = 0, \text{ for } j \in \mathcal{I}. \end{aligned}$$

On the whole metric graph one considers again the direct sums of these spaces

$$\mathcal{D} \equiv \mathcal{D}(\mathcal{E}, \mathcal{I}) = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{D}_j, \quad \text{and} \quad \mathcal{D}^0 \equiv \mathcal{D}^0(\mathcal{E}, \mathcal{I}) = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{D}_j^0. \tag{6}$$

Note that these spaces clearly decouple the edges of the graph. With the scalar products $\langle\cdot,\cdot\rangle_{\mathcal{W}}$ defined by

$$\langle\varphi, \psi\rangle_{\mathcal{W}} = \langle\varphi, \psi\rangle_{\mathcal{H}} + \langle\varphi', \psi'\rangle_{\mathcal{H}}$$

and $\langle\cdot,\cdot\rangle_{\mathcal{D}}$ given by

$$\langle\varphi, \psi\rangle_{\mathcal{D}} = \langle\varphi, \psi\rangle_{\mathcal{H}} + \langle\varphi', \psi'\rangle_{\mathcal{H}} + \langle\varphi'', \psi''\rangle_{\mathcal{H}}$$

the spaces $\mathcal{W}$ and $\mathcal{D}$, respectively become themselves Hilbert spaces.

The Hilbert space

$$\mathcal{H}^2 \equiv \mathcal{H}^2(\mathcal{E},\mathcal{I},\underline{a}) = \mathcal{H}^2_{\mathcal{E}} \oplus \mathcal{H}^2_{\mathcal{I}}, \quad \mathcal{H}^2_{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \mathcal{H}^2_e, \quad \mathcal{H}^2_{\mathcal{I}} = \bigoplus_{i\in\mathcal{I}} \mathcal{H}^2_i, \tag{7}$$

where $\mathcal{H}^2_j = L^2(I_j;\mathbb{C}^2)$ is considered also. Note that any function $\psi_j \in \mathcal{H}^2_j$ can be written as vector valued function

$$\psi_j = \begin{bmatrix} \psi_j^1 \\ \psi_j^2 \end{bmatrix}.$$

By $\mathcal{W}^2_j$ one denotes the set of all $\psi_j \in \mathcal{H}^2_j$ such that ψ_j is absolutely continuous and ψ_j' is square integrable. Let $\mathcal{W}^2_{j,0}$ denote the set of all those elements $\psi_j \in \mathcal{W}^2_j$ with

$$\begin{aligned} &\psi_j^1(0) = 0, \quad \psi_j^2(0) = 0, \quad \text{for } j \in \mathcal{E}, \\ &\psi_j^1(0) = 0, \quad \psi_j^2(0) = 0, \quad \psi_j^1(a_j) = 0,\ \psi_j^2(a_j) = 0,\ \text{for } j \in \mathcal{I}. \end{aligned}$$

On the whole metric graph one considers the direct sums

$$\mathcal{W}^2 \equiv \mathcal{W}^2(\mathcal{E},\mathcal{I}) = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{W}^2_j, \quad \text{and} \quad \mathcal{W}^2_0 \equiv \mathcal{W}^2_0(\mathcal{E},\mathcal{I}) = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{W}^2_{j,0}. \tag{8}$$

Differential operators. The probably most studied operator on metric graphs is the Laplace operator. The subject of Laplace operators on metric graphs has attracted a lot of attention in the last decades. Without going into details I would like to refer to the works [14, 60, 71, 72] and the references therein, where also a brief overview on the history of the different branches of the development and their applications can be found.

Let Δ be the differential operator defined by

$$(\Delta\psi)_j(x) = \frac{d^2}{dx}\psi_j(x), \quad j \in \mathcal{E}\cup\mathcal{I}, \quad x \in I_j \tag{9}$$

with domain $\mathcal{D}$ and let Δ^0 be its restriction to the domain $\mathcal{D}^0$. Then $-\Delta^0$ is a non–negative closed symmetric operator. The appropriate objects to measure how far a closed symmetric operator is from being self–adjoint are the deficiency indices

$$d_\pm = \dim \operatorname{Ker}\left(\left(\Delta^0\right)^* \pm i \right).$$

These are elements of the classical theory of extensions of symmetric operators, see for example the books [18], [37] and [92] for a presentation of this subject. The Hilbert space adjoint of Δ^0 is

$$\Delta = \left(\Delta^0\right)^*.$$

The operator Δ^0 has equal deficiency indices $(d_+, d_-) = (d, d)$, where $d = |\mathcal{E}| + 2|\mathcal{I}|$. It is crucial to note that extensions $\widetilde{\Delta}$ of Δ^0 with

$$\Delta^0 \subset \widetilde{\Delta} \subset \Delta$$

can be studied in terms of boundary conditions, compare for example [47, 60]. Properties of certain extensions of the minimal Laplace operator $-\Delta^0$ are discussed in the following two chapters. In Chapters 1 the question of quasi–m–accretive and of m–accretive extensions is discussed and in Chapter 2 estimates on the negative eigenvalues of self–adjoint Laplacians are derived.

Dirac operators on metric graphs have attracted interest too, and they have been studied intensely, compare for example [20, 80]. The (maximal) Dirac operator D is defined by

$$(D\psi)_j(x) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \frac{d}{dx}\psi_j(x), \quad j \in \mathcal{E}\cup\mathcal{I}, \quad x \in I_j \tag{10}$$

on the domain $\mathcal{W}^2$ and the (minimal) Dirac operator D^0 is its restriction to $\mathcal{W}_0^2$. The operator D^0 is a closed symmetric operator with equal deficiency indices $(|\mathcal{E}|+2|\mathcal{I}|, |\mathcal{E}|+2|\mathcal{I}|)$. However, it is not semi–bounded.

In Chapter 3 another type of differential operator is considered. On a compact metric graph $(\mathcal{G}, \underline{a})$, $\mathcal{G} = (V, \mathcal{I}, \partial)$, with subdivision of its internal edges

$$\mathcal{I} = \mathcal{I}_d \dot{\cup} \mathcal{I}_t$$

the operator A is defined on each edge by

$$(A\psi)_j(x) = \begin{cases} +\frac{d^2}{dx}\psi_j(x), & j \in \mathcal{I}_d,\ x \in I_j, \\ -\frac{d}{dx}\psi_j(x), & j \in \mathcal{I}_t,\ x \in I_j, \end{cases}$$

for $\psi \in \operatorname{Dom}(A) = \mathcal{D}(\mathcal{I}_d) \oplus \mathcal{W}(\mathcal{I}_t)$. A natural minimal operator A^0 is given by the restriction of A to $\operatorname{Dom}(A^0) = \mathcal{D}^0(\mathcal{I}_d) \oplus \mathcal{W}^0(\mathcal{I}_t)$. Note that the operator A^0 is the direct sum of a symmetric and a skew–symmetric operator. Here, a class of quasi–m–dissipative extensions with domain lying between this minimal and the maximal domain is studied.

Similarly, a generalization of the operator

$$-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$$

to metric graphs is introduced in Chapter 4 using the differential expression τ defined by

$$(\tau\psi)_j(x) = \begin{cases} +\frac{d^2}{dx}\psi_j(x), & j \in \mathcal{I}_- \cup \mathcal{E}_-,\ x \in I_j, \\ -\frac{d^2}{dx}\psi_j(x), & j \in \mathcal{I}_+ \cup \mathcal{E}_+,\ x \in I_j, \end{cases}$$

where one differentiates between positive edges $\mathcal{E}_+ \cup \mathcal{I}_+$ and negative edges $\mathcal{E}_- \cup \mathcal{I}_-$ with

$$\mathcal{E} = \mathcal{E}_+ \cup \mathcal{E}_- \quad \text{and} \quad \mathcal{I} = \mathcal{I}_+ \cup \mathcal{I}_-.$$

The minimal and the maximal domains are the same as for the Laplace operator and it is going to turn out that there is a tight relation between self–adjoint extensions of the Laplacian and self–adjoint realisations of τ.

Spaces of boundary values. One is interested in couplings taking place at vertices. It has turned out, roughly speaking, that it is easier to glue together functions defined on separated intervals rather than to glue together the underlying spaces and then to define appropriate function spaces. Therefore the coupling between the functions on different edges is implemented in terms of boundary or matching conditions imposed at the endpoints of the edges. For this purpose one needs boundary values or traces of certain functions.

For $\psi \in \mathcal{D}$ one defines the vectors of boundary values

$$\underline{\psi} = \begin{bmatrix} \{\psi_e(0)\}_{e\in\mathcal{E}} \\ \{\psi_i(0)\}_{i\in\mathcal{I}} \\ \{\psi_i(a_i)\}_{i\in\mathcal{I}} \end{bmatrix} \quad \text{and} \quad \underline{\psi}' = \begin{bmatrix} \{\psi_e'(0)\}_{e\in\mathcal{E}} \\ \{\psi_i'(0)\}_{i\in\mathcal{I}} \\ \{-\psi_i'(a_i)\}_{i\in\mathcal{I}} \end{bmatrix}. \tag{11}$$

One introduces the auxiliary Hilbert space

$$\mathcal{K} \equiv \mathcal{K}(\mathcal{E},\mathcal{I}) = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^{-} \oplus \mathcal{K}_{\mathcal{I}}^{+} \tag{12}$$

with $\mathcal{K}_{\mathcal{E}} \cong \mathbb{C}^{|\mathcal{E}|}$ and $\mathcal{K}_{\mathcal{I}}^{(\pm)} \cong \mathbb{C}^{|\mathcal{I}|}$, and one sets

$$[\psi] := \underline{\psi} \oplus \underline{\psi}' \in \mathcal{K} \oplus \mathcal{K}.$$

The redoubled space $\mathcal{K}^2 = \mathcal{K} \oplus \mathcal{K}$ is denoted *space of boundary values*. For $\psi \in \mathcal{W}$ the trace $\underline{\psi}$ is still well–defined. Suitable matching conditions, appropriate traces and domains of definitions for the various differential operators are discussed in the correspondent chapters.

CHAPTER 1

Quasi–m–accretive Laplace operators

This chapter is devoted to the study of quasi–m–accretive Laplace operators on finite metric graphs. For a finite not necessarily compact metric graph, one considers the differential expression $-\frac{d^2}{dx^2}$ on each edge. The boundary conditions at the vertices of the graph that yield quasi–m–accretive as well as those that give m–accretive realizations are completely characterized. This solves the problem of the well–posedness of the initial value problem for the diffusion equation on metric graphs, because the infinitesimal generators of quasi–contractive semigroups are exactly minus the quasi–m–accretive operators. The content of this chapter is also available as preprint, see [51].

Recall that an operator T acting in a Hilbert space $\mathcal{H}$ with scalar product $\langle\cdot,\cdot\rangle$ is called *quasi–accretive* if there exists a real constant C such that

$$\operatorname{Re}\langle u, Tu\rangle + C\langle u, u\rangle \geq 0, \quad \text{for all } u \in \operatorname{Dom}(T).$$

The operator T is called *accretive* if C can be chosen to be zero.

In the literature there are several equivalent definitions for the notion of (quasi–)m–accretive operators. Here the following is proposed: A closed (quasi–)accretive operator is *(quasi–)m–accretive* if it has no proper (quasi–)m–accretive extension. In this sense (quasi–)m–accretive operators are maximal (quasi–)accretive. This is basically the notion used by V. Kostrykin and R. Schrader in [64]. Note that a closed operator T is m–accretive if and only if

$$\{\lambda \in \mathbb{C} \mid \operatorname{Re}\lambda > 0\} \subset \rho(T),$$

where $\rho(T)$ is the resolvent set of T, and it obeys the estimate

$$\|(T-\lambda)^{-1}\| \leq (\operatorname{Re}\lambda)^{-1} \quad \text{for } \operatorname{Re}\lambda > 0,$$

compare [58, Chapter V, §3.10], where this has been used actually as definition for m–accretivity, and in the references given there the equivalence to the above definition is stated. An operator is quasi–m–accretive if $T - C$ is accretive for some C. While the above conditions can be sometimes hard to verify directly, it is known that a closed operator T is (quasi–)m–accretive if and only if both T and its adjoint T^* are quasi–accretive. Equivalently, a closed and densely defined operator T is (quasi–)m–accretive if $T - C$ is accretive with some constant C, and there is a $\lambda < C$ such that $T - \lambda$ is surjective. An operator L is called *(quasi–)dissipative* if the operator $T = -L$ is (quasi–)accretive, and L is called *(quasi–)m–dissipative* if the operator $T = -L$ is (quasi–)m–accretive.

Let be $C \in \mathbb{R}$, then the operator T is called *sectorial with vertex* C, if

$$|\operatorname{Im}\langle u, Tu\rangle| \leq \operatorname{Re}\langle u, Tu\rangle + C\langle u, u\rangle, \quad \text{for all } u \in \operatorname{Dom}(T).$$

An operator T is called *sectorial* if it is sectorial with some vertex C. Furthermore, a closed sectorial operator T is called *m–sectorial* if it is in addition quasi–m–accretive, compare [58, Chapter V, §3.10].

Note that the notions (quasi–)accretive and sectorial are referring to the numerical range

$$\mathcal{N}(T) = \{\langle u, Tu\rangle \mid u \in \operatorname{Dom}(T) \text{ with } \|u\| = 1\} \subset \mathbb{C}$$

of a closed operator T rather than to its spectrum,

$$\sigma(T) = \{\lambda \in \mathbb{C} \mid (T - \lambda) \text{ boundedly invertible}\} \subset \mathbb{C}.$$

In general the numerical range can be much larger than the convex hull of the spectrum, see for instance [88, Example 1.3.3] for an illustrative example.

A semigroup $(S(t))_{t\geq 0}$ is strongly continuous and (quasi)–contractive if and only if its infinitesimal generator L is (quasi)–m–dissipative and then $S(t) = e^{Lt}$, see for example [33, Chapter II Corollary 3.6]. Recall that a strongly continuous semigroup $(S(t))_{t\geq 0}$ is called *quasi–contractive* if

$$\|S(t)\| \leq e^{\omega t}$$

for appropriate $\omega \in \mathbb{R}$, see for example [33, Chapter II Corollary 3.6]. The growth bound ω can be chosen as $\omega = \inf \operatorname{Re} \mathcal{N}(-L)$, where L is the quasi–m–dissipative generator of $(S(t))_{t\geq 0}$, see [33, Chapter II Corollary 3.6] along with [58, Chapter V, §10]. If $\|S(t)\| \leq 1$ holds for $t \geq 0$ the semigroup $(S(t))_{t\geq 0}$ is called *contractive*.

The scope of this chapter is the heat conduction equation on finite metric graphs with initial conditions. So, let be given a finite metric graph $(\mathcal{G}, \underline{a})$, and for a Laplace operator $-\widetilde{\Delta}$ in $\mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a})$ with $-\Delta^0 \subset -\widetilde{\Delta}$ one considers the Cauchy problem

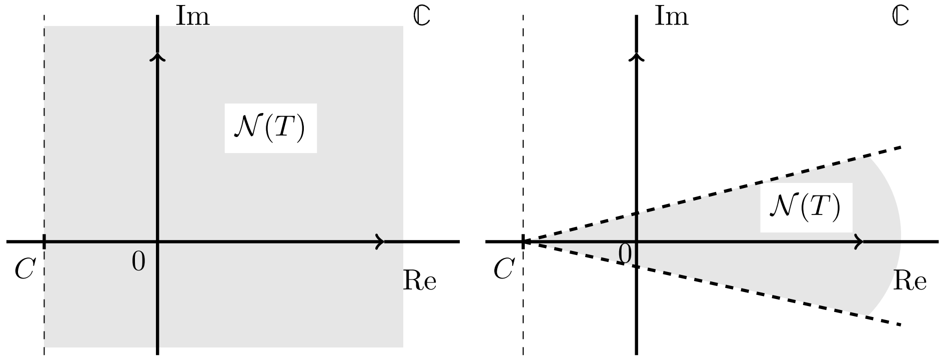
$$\begin{cases} \left(\dfrac{\partial}{\partial t} - \widetilde{\Delta}\right) \psi(x,t) = 0, \\ \\ \psi(\cdot, 0) = \psi_0, \quad \text{for } t \geq 0. \end{cases} \tag{13}$$

The quasi–m–accretive Laplace operators $-\widetilde{\Delta}$ give exactly the quasi–m–dissipative generators $\widetilde{\Delta}$ of strongly continuous and quasi–contractive semigroups. Hence, for $-\widetilde{\Delta}$ quasi–m–accretive the solution of the Cauchy problem (13) in the space $\mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a})$, is given in terms of semigroups by

$$\psi(\cdot, t) = e^{\widetilde{\Delta} t}\psi_0, \quad \text{where} \quad \|e^{\widetilde{\Delta} t}\| \leq e^{\omega t},$$

for appropriate growth bound $\omega \in \mathbb{R}$. In particular, this has applications to stochastic processes on networks. For further information on this subject, especially on Brownian motions on metric graphs, see [64–68].

The present work can be understood as an extension of the results obtained by V. Kostrykin and R. Schrader in the article [64], where a sufficient criterion for m–accretive boundary conditions has been derived. In particular, there it has been stated that all m–accretive Laplacians can be parametrized in terms of boundary conditions. The main statement here is the characterization of all quasi–m–accretive Laplacians on finite metric graphs in terms of boundary conditions. Furthermore the proof shows that these Laplacians are even m–sectorial and that their real parts are self–adjoint Laplace operators. Combining the main result with results from [12] on non–negative self–adjoint Laplacians on finite metric graphs, one obtains also a complete characterization of all m–accretive boundary conditions.



(a) Numerical range of a quasi–accretive operator T.

(b) Numerical range of an operator T that is sectorial with vertex C.

FIGURE 1. Quasi–accretive and sectorial operators.

The subject of Laplacians on metric graphs lies - from the mathematical point of view - in the intersection of different branches of mathematics. Here it is worth mentioning spectral theory and the theory of ordinary differential equations or systems of them. One approach is to put the question of appropriate boundary conditions into the framework of extension theory. In the most general context of extension theory results characterising m–accretive extensions of non–negative closed symmetric operators have been obtained by Y. Arlinskii, Y. Kovalev and È. R. Tsekanovskiĭ, compare the recent work [7] and the references therein. In the more specific context of boundary triples V. A. Derkach, M. M. Malamud and È. R. Tsekanovskiĭ, see [30] and M. M. Malamud, see [74], obtained characterizations earlier. The question of quasi–self–adjoint Laplace operators on graphs discussed here can also be transferred into the context of boundary triples, compare [12] and the references given therein, and by applying the above mentioned results one can obtain a characterisation of all (quasi–)m–accretive boundary conditions as well. Here, the intention is to give an elementary proof of this characterisation which also might furnish a good understanding of the matter.

This chapter is organized as follows: in the subsequent section the different types of boundary conditions are discussed and the starting point of the study is described. This is followed by the formulation of the main results and the discussion of examples. The proofs are given separately in the last section.

1.1. Boundary conditions

Let $(\mathcal{G},\underline{a})$ be a finite metric graph. The aim of this chapter is to discuss extensions $-\widetilde{\Delta}$ of the Laplacian $-\Delta^0$ that lie between the minimal and the maximal operator, that is

$$-\Delta^0 \subset -\widetilde{\Delta} \subset -\Delta.$$

In the context of extension theory, extensions with this property are called *quasi–self–adjoint*, compare for instance [7]. In the situation considered here these extensions can be discussed in terms of boundary conditions imposed at the vertices of the graph. For this purpose one considers the auxiliary Hilbert space

$$\mathcal{K} \equiv \mathcal{K}(\mathcal{E},\mathcal{I}) = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^{-} \oplus \mathcal{K}_{\mathcal{I}}^{+}$$

defined in (12). Recall that for $\psi \in \mathcal{D}$ the vectors of boundary values are

$$\underline{\psi} = \begin{bmatrix} \{\psi_e(0)\}_{e\in\mathcal{E}} \\ \{\psi_i(0)\}_{i\in\mathcal{I}} \\ \{\psi_i(a_i)\}_{i\in\mathcal{I}} \end{bmatrix}, \qquad \underline{\psi}' = \begin{bmatrix} \{\psi_e'(0)\}_{e\in\mathcal{E}} \\ \{\psi_i'(0)\}_{i\in\mathcal{I}} \\ \{-\psi_i'(a_i)\}_{i\in\mathcal{I}} \end{bmatrix}$$

and

$$[\psi] := \underline{\psi} \oplus \underline{\psi}' \in \mathcal{K} \oplus \mathcal{K}$$

is an element in the space of boundary values.

Let A and B be linear maps in $\mathcal{K}$. By $(A,\, B)$ one denotes the linear map from $\mathcal{K}^2 = \mathcal{K} \oplus \mathcal{K}$ to $\mathcal{K}$ defined by

$$(A,\, B)(\chi_1 \oplus \chi_2) = A\chi_1 + B\chi_2$$

with $\chi_1, \chi_2 \in \mathcal{K}$. Set

$$\mathcal{M}(A, B) := \operatorname{Ker}(A,\, B). \tag{14}$$

With any subspace $\mathcal{M} \subset \mathcal{K}^2$ one can associate an extension $-\Delta(\mathcal{M})$ of $-\Delta^0$, which is the restriction of $-\Delta$ to the domain

$$\operatorname{Dom}(-\Delta(\mathcal{M})) = \{\psi \in \mathcal{D} \mid [\psi] \in \mathcal{M}\}.$$

If $\mathcal{M} = \mathcal{M}(A, B)$ is of the form given in (14) an equivalent description is that $\operatorname{Dom}(-\Delta(\mathcal{M}))$ consists of all functions $\psi \in \mathcal{D}$ satisfying the linear boundary conditions

$$A\underline{\psi} + B\underline{\psi}' = 0.$$

In this case one writes equivalently $-\Delta(\mathcal{M}) = -\Delta(A, B)$.

In [64, Theorem 2.3] it is shown that each m–accretive extension of $-\Delta^0$ can be represented as $-\Delta(A, B)$, for some A and B satisfying the following necessary

ASSUMPTION 1.1 ([64, Assumption 2.1]). *Let A and B be maps in $\mathcal{K}$. Assume that the map $(A,\, B)\colon \mathcal{K}^2 \to \mathcal{K}$ is surjective, that is, it has maximal rank equal to $d = |\mathcal{E}| + 2|\mathcal{I}|$.*

The statement of [64, Theorem 2.3] admits a straight forward generalization to quasi–m–accretive Laplacians.

PROPOSITION 1.2. *Any quasi–m–accretive extension of $-\Delta^0$ can be represented by $-\Delta(A, B)$, for some A and B satisfying Assumption 1.1.*

The proof is completely analogous to the one of [64, Theorem 2.3] and it is omitted here.

For the discussion of boundary conditions it is important to note that A, B and A', B' define the same operator $-\Delta(A, B) = -\Delta(A', B')$ if and only if the corresponding subspaces $\mathcal{M}(A, B)$ and $\mathcal{M}(A', B')$ agree. This gives rise to

DEFINITION 1.3 ([64, Definition 2.2]). *Boundary conditions defined by A, B and A', B' satisfying Assumption 1.1 are called equivalent if the corresponding subspaces $\mathcal{M}(A, B)$ and $\mathcal{M}(A', B')$ agree.*

Note that boundary conditions defined by A, B and A', B' satisfying Assumption 1.1 are equivalent if and only if there exists an invertible operator C in $\mathcal{K}$ such that $A' = CA$ and $B' = CB$, compare also [64].

The question if an operator is quasi–accretive or even sectorial is closely related to the sesquilinear form defined by the operator, and here one defines the sesquilinear form $\delta_{\mathcal{M}}$ by

$$\delta_{\mathcal{M}}[\psi,\varphi] := \langle \psi, -\Delta(\mathcal{M})\varphi\rangle_{\mathcal{H}}, \quad \psi,\varphi \in \mathrm{Dom}(\Delta(\mathcal{M})).$$

Integration by parts gives a more practical representation for the associated quadratic form

$$\delta_{\mathcal{M}}[\psi] := \delta_{\mathcal{M}}[\psi,\psi] = \int_{\mathcal{G}} |\psi'|^2 + \langle \underline{\psi}, \underline{\psi}'\rangle_{\mathcal{K}}. \tag{15}$$

It turns out that within the class of boundary conditions which satisfy Assumption 1.1, one can distinguish two types of boundary conditions. These are related to a certain block decomposition of the matrices A and B. Following [72, Section 3.1] one introduces two decompositions of $\mathcal{K}$. Denote by Q the orthogonal projector onto $(\mathrm{Ran}\, B)^{\perp}$, by $Q^{\perp} = \mathbb{1} - Q$ the orthogonal projector onto $\mathrm{Ran}\, B$ and by P the orthogonal projector onto $\mathrm{Ker}\, B$ and by $P^{\perp} = \mathbb{1} - P$ the orthogonal projector onto $(\mathrm{Ker}\, B)^{\perp}$. With this one is able to write the map $(A,\, B)$ as the block operator matrix

$$(A,\, B) = \begin{pmatrix} Q^{\perp}AP^{\perp} & Q^{\perp}AP & Q^{\perp}BP^{\perp} & 0 \\ QAP^{\perp} & QAP & 0 & 0 \end{pmatrix}. \tag{16}$$

The domains of A and B have the orthogonal decomposition $\mathcal{K} = \mathrm{Ran}\, P \oplus \mathrm{Ran}\, P^{\perp}$ and the target set of both A and B is $\mathcal{K} = \mathrm{Ran}\, Q \oplus \mathrm{Ran}\, Q^{\perp}$. From this one sees that the rank condition in Assumption 1.1 is equivalent to the fact that $QA = \begin{bmatrix} QAP^{\perp} & QAP \end{bmatrix}$ considered as a map from $\mathcal{K}$ to $\mathrm{Ran}\, Q$ is surjective.

As remarked above, the choice of the matrices A and B is not unique. Similar to the case of self–adjoint Laplace operators, on metric graphs one can parametrize the space $\mathcal{M}$ at least in an "almost unique" way. Notice that it follows from the definitions of P and Q that $\dim \mathrm{Ran}\, P = \dim \mathrm{Ran}\, Q$. Therefore there exists an isomorphism

$$U\colon\ \mathrm{Ran}\, Q \to \mathrm{Ran}\, P.$$

Multiplying both A and B from the left with the diagonal block operator matrix

$$C = \begin{bmatrix} (Q^{\perp}BP^{\perp})^{-1} & 0 \\ 0 & U \end{bmatrix},$$

gives $A' = CA$ and $B' = CB$. These A', B' define equivalent boundary conditions in the sense of Definition 1.3, that is $\mathcal{M}(A', B') = \mathcal{M}(A, B)$, but one has achieved the normalization $B' = P^{\perp}$. This gives the block operator matrix representation

$$(A',\, B') = \begin{pmatrix} P^{\perp}A'P^{\perp} & P^{\perp}A'P & P^{\perp} & 0 \\ PA'P^{\perp} & PA'P & 0 & 0 \end{pmatrix}. \tag{17}$$

One observes that these boundary conditions can be separated into

$$PA'\underline{\psi} = 0 \quad \text{and} \quad P^{\perp}A'\underline{\psi} + P^{\perp}\underline{\psi}' = 0.$$

Similar considerations have been used in the article [72] for the discussion of boundary conditions that define self–adjoint Laplace operators as well as in the analysis of the corresponding quadratic forms. This motivates the notation

$$L := (Q^{\perp}BP^{\perp})^{-1}Q^{\perp}AP^{\perp} \tag{18}$$

or equivalently $L = P^{\perp}A'P^{\perp}$. After this preparatory work one can formulate also the sufficient assumption on boundary conditions to define quasi–m–accretive realisations of $-\Delta$. In addition to the necessary Assumption 1.1 one needs

ASSUMPTION 1.4. *Let A and B be maps in $\mathcal{K}$. Let Q be the orthogonal projector in $\mathcal{K}$ onto $(\operatorname{Ran} B)^{\perp}$, P the orthogonal projector in $\mathcal{K}$ onto $\operatorname{Ker} B$ and $P^{\perp} = \mathbb{1} - P$ the complementary projector. Assume that*

$$QAP^{\perp} = 0.$$

REMARK 1.5. *Assuming both Assumption 1.1 and Assumption 1.4 it follows that QAP, as a map from $\operatorname{Ran} P$ to $\operatorname{Ran} Q$ is invertible. With this the block–decomposition given in* (17) *can be simplified to become*

$$(A',\, B') = \begin{pmatrix} P^{\perp}A'P^{\perp} & P^{\perp}A'P & P^{\perp} & 0 \\ 0 & P & 0 & 0 \end{pmatrix}. \tag{19}$$

The block $P^{\perp}A'P$ has no influence on the domain of $-\Delta(A', B')$, since $P\underline{\psi} = 0$ for all $\psi \in \operatorname{Dom}(-\Delta(A', B'))$. Hence, one can consider equivalently

$$(A'',\, B'') = \begin{pmatrix} L & 0 & P^{\perp} & 0 \\ 0 & P & 0 & 0 \end{pmatrix}. \tag{20}$$

1.2. Characterizations and examples

The main result of this chapter is

THEOREM 1.6.

(1) The operator $-\Delta(A, B)$ is quasi–m–accretive if and only if A, B satisfy both Assumption 1.1 and Assumption 1.4.

(2) Any quasi–m–accretive Laplace operator $-\Delta(A, B)$ is m–sectorial and associated with the form defined by

$$\int_{\mathcal{G}} |\psi'|^2 - \langle LP^{\perp}\underline{\psi}, P^{\perp}\underline{\psi}\rangle_{\mathcal{K}}, \quad \psi \in \{\varphi \in \mathcal{W} \mid P\underline{\varphi} = 0\},$$

where P is the orthogonal projector onto $\operatorname{Ker} B$, $P^{\perp} = \mathbb{1} - P$ is its complementary projector and L is computed from A, B by formula (18). *In particular, its real part*

$$\operatorname{Re}(-\Delta(A, B)) = -\Delta(A', B'),$$

is a self–adjoint Laplace operator, where

$$A' = P + \operatorname{Re} L \quad \textit{and} \quad B' = P^{\perp}.$$

Note that for any positive closed symmetric operator with equal and non–zero deficiency indices there exists an extension that is m–accretive, but not sectorial with vertex zero, see [89, Theorem 1]. In the particular situation considered here statement (2) of Theorem 1.6 exhibits that there is at least some vertex for which the m–accretive operator $-\Delta(A, B)$ is sectorial. This is of importance because the first representation theorem applies to m–sectorial operators, and any m–sectorial operator $-\Delta(A, B)$ has a well–defined real part $\operatorname{Re}(-\Delta(A, B))$. This is the unique self–adjoint operator that is associated to the real part of the closure of the form defined by the m–sectorial operator $-\Delta(A, B)$, compare [58, Chapter VI, §3.1]. In particular $\operatorname{Re}(-\Delta(A, B))$ is itself a Laplace operator. Combining [12, Theorem 1] with the above Theorem 1.6 yields also a characterisation of all m–accretive boundary conditions.

THEOREM 1.7. *The operator $-\Delta(A,B)$ is m–accretive if and only if Assumption 1.1 holds and*

$$\operatorname{Re}(AB^*) + BM_0(\underline{a})B^* \leq 0 \quad \text{with } M_0(\underline{a}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{1}{\underline{a}} & \frac{1}{\underline{a}} \\ 0 & \frac{1}{\underline{a}} & -\frac{1}{\underline{a}} \end{pmatrix},$$

where $\frac{1}{\underline{a}}$ is the $|\mathcal{I}| \times |\mathcal{I}|$–matrix with entries $\left\{\frac{1}{\underline{a}}\right\}_{ij} = \delta_{ij} a_i^{-1}$, $i,j \in \mathcal{I}$.

This theorem improves the result obtained in [64, Theorem 2.4], where it has been stated that boundary conditions A,B satisfying Assumption 1.1 define an m–accretive Laplace operator $-\Delta(A,B)$ whenever $\operatorname{Re}(AB^*) \leq 0$. This follows now already from the inequality

$$\operatorname{Re}(AB^*) + BM_0(\underline{a})B^* \leq \operatorname{Re}(AB^*)$$

which makes use of $BM_0(\underline{a})B^* \leq 0$. Note that the condition $\operatorname{Re}(AB^*) + BM_0(\underline{a})B^* \leq 0$ in Theorem 1.7 assures that Assumption 1.4, which is needed to apply Theorem 1.6, is satisfied.

The statement of Theorem 1.7 follows as well from the more general results obtained in [30, Theorem 2] for boundary triples. Applying [30, Theorem 2] to operators $-\Delta(A,B)-C$ for $C > 0$ and combining this with the forthcoming Lemma 1.16 one can also prove the characterisation of all quasi–m–accretive boundary conditions stated in Theorem 1.6.

REMARK 1.8. *Quasi–m–accretive operators $-\Delta(A,B)$ generate strongly continuous quasi–contractive semigroups given by*

$$S(t) = e^{t\Delta(A,B)} \quad \text{with growth estimate} \quad \|S(t)\| \leq e^{-t\omega},$$

where the growth bound ω can be chosen as

$$\omega = \inf \operatorname{Re}\{\langle \psi, -\Delta(A,B)\psi\rangle \mid \psi \in \operatorname{Dom}(-\Delta(A,B)),\ \|\psi\| = 1\}.$$

This follows from [33, Chapter II Corollary 3.6] and [58, Chapter V, §10]. Therefore the growth bound ω can be computed, according to Theorem 1.7, as the bottom of the spectrum of the self–adjoint operator $-\Delta(A',B') = -\operatorname{Re}\Delta(A,B)$ by

$$\omega = \min \sigma(-\Delta(A',B')).$$

Two–sided estimates on the lowest negative eigenvalue of a self–adjoint Laplacian on a finite metric graph are discussed in Chapter 2 of this work.

Note that all boundary conditions A,B satisfying Assumption 1.1 with $\operatorname{Ker} B = 0$, satisfy also Assumption 1.4 since then $L = B^{-1}A$ and $P = 0$. Separated boundary conditions on intervals are of this type as well as the conditions given in the next but one example, whereas the next example gives quasi–m–accretive boundary conditions with $P \neq 0$.

EXAMPLE 1.9 (Complex δ-interaction). *Assume that the boundary conditions are local and for* $\deg(\nu) \geq 2$ *the boundary conditions at vertex* ν *are defined up to equivalence by*

$$A_\nu = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & \gamma_\nu \end{bmatrix}, \qquad B_\nu = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1 \end{bmatrix},$$

where $\gamma_\nu \in \mathbb{C}$. *For real* γ_ν *the Assumptions 1.1 and 1.4 are satisfied, that is one can represent the boundary conditions equivalently by* $A'_\nu = L_\nu + P_\nu$ *and* $B'_\nu = P_\nu^\perp$, *where* $P_\nu^\perp$ *is the rank one projector onto* $(\operatorname{Ker} B_\nu)^\perp$ *and* $L_\nu = \frac{-\gamma_\nu}{\deg(\nu)} P_\nu^\perp$, *compare [72, Section 3.2.1]. A direct calculation shows that this carries over to the case of complex coupling parameters* γ_ν, *and consequently Assumptions 1.1 and 1.4 are satisfied. For a connected star graph with complex* δ*-interaction at the central vertex with coupling constant* γ_ν *the operator* $-\Delta(A_\nu, B_\nu)$ *is associated with the quadratic form defined by*

$$\int_{\mathcal{G}} |\psi'|^2 - \frac{\gamma_\nu}{\deg(\nu)} |\underline{\psi}|^2, \quad \textit{where } \psi \in \{\psi \in \mathcal{W} \mid P_\nu \underline{\psi} = 0\},$$

and hence $\operatorname{Re}(-\Delta(A_\nu, B_\nu))$ *is the self–adjoint Laplace operator with real* δ*-interaction and coupling parameter* $\operatorname{Re}\gamma_\nu$ *at the vertex.*

EXAMPLE 1.10 (Complex δ'–interaction). *Let the boundary conditions be local. A type of complex* δ'*–interaction is given for* $\gamma_\nu \in \mathbb{C} \setminus \{0\}$ *by* $\hat{A}_\nu = B_\nu$ *and* $\hat{B}_\nu = A_\nu$, *where* A_ν *and* B_ν *are taken from the above Example 1.9, compare [72, Section 3.2.3] for the case of real coupling constant. Since* $\hat{B}_\nu$ *is invertible one has*

$$\hat{L}_\nu = \hat{B}_\nu^{-1} \hat{A}_\nu \quad \textit{and} \quad \hat{P}_\nu = 0.$$

Consequently, Assumptions 1.1 and 1.4 are satisfied, and hence these boundary conditions define quasi–m–accretive Laplace operators. Note that $\hat{L}_\nu$ *is a rank one operator, and* $\operatorname{Re}(-\Delta(\hat{A}_\nu, \hat{B}_\nu))$ *is the self–adjoint Laplace operator with* δ'*–interactions and coupling parameters* $\operatorname{Re}\gamma_\nu$.

An example for which Assumption 1.1 is satisfied, but Assumption 1.4 is violated is the following

EXAMPLE 1.11. *Let* $\mathcal{G} = (V, \partial, \mathcal{E})$ *be a graph consisting of two external edges* $\mathcal{E} = \{e_1, e_2\}$ *and one vertex* $\partial(e_1) = \partial(e_2)$. *Consider the boundary conditions defined by*

$$A_\tau = \begin{bmatrix} 1 & -e^{i\tau} \\ 0 & 0 \end{bmatrix} \quad \textit{and} \quad B_\tau = \begin{bmatrix} 0 & 0 \\ 1 & -e^{-i\tau} \end{bmatrix},$$

for $\tau \in [0, \pi/2]$. *Assumption 1.1 is clearly satisfied for any* $\tau \in [0, \pi/2]$. *Explicit computations give*

$$\operatorname{Ran} B_\tau = \operatorname{span}\left\{ \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}, \qquad (\operatorname{Ran} B_\tau)^\perp = \operatorname{span}\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right\},$$

$$\operatorname{Ker} B_\tau = \operatorname{span}\left\{ \begin{bmatrix} e^{-i\tau} \\ 1 \end{bmatrix} \right\}, \qquad (\operatorname{Ker} B_\tau)^\perp = \operatorname{span}\left\{ \begin{bmatrix} 1 \\ -e^{-i\tau} \end{bmatrix} \right\}$$

and therefore

$$Q_\tau A_\tau P_\tau^\perp = \frac{1}{\sqrt{2}}\begin{bmatrix} 2 & -2e^{i\tau} \\ 0 & 0 \end{bmatrix} \neq 0.$$

The case $\tau = 0$ is closely related to the boundary conditions discussed in [32, Example XIX.6.c]. The function $\psi(k,\cdot)$ defined by

$$\psi(k,x) = \begin{cases} e^{ikx}, & x \in e_1, \\ e^{ikx}, & x \in e_2 \end{cases}$$

satisfies the boundary conditions defined by A_0 and B_0 for any k. For any $\operatorname{Im} k > 0$ one has

$$-\Delta(A_0,B_0)\psi(k,\cdot) = k^2\psi(k,\cdot),$$

and hence the operator $-\Delta(A_0,B_0)$ has empty resolvent set. Identifying the metric graph $\mathcal{G}$ with the real line one obtains that the operator $-\Delta(A_0,B_0)$ on $\mathcal{G}$ corresponds to the operator

$$-\operatorname{sign}(x)\tfrac{d}{dx}\operatorname{sign}(x)\tfrac{d}{dx}$$

with its natural domain in $L^2(\mathbb{R};\mathbb{C})$. Note that the operator $-\Delta(A_0,B_0)$ is self–adjoint in a certain Krein space, see Proposition 4.8 in Chapter 4 and the following. As it has empty resolvent set it cannot be similar to a self–adjoint operator in the Hilbert space $\mathcal{H}$.

Similar examples are studied in the context of $\mathcal{PT}$–symmetry, see for instance [85] and the references quoted therein.

1.3. Proofs of the main results

The proofs of the characterizations consist of two directions. For the "if–part" one requires both Assumptions 1.1 and 1.4. Recall that a form $\mathfrak{t}$ is called *sectorial* if there exists a $C \in \mathbb{R}$ such that

$$|\operatorname{Im}\mathfrak{t}[u,u]| \leq \operatorname{Re}\mathfrak{t}[u,u] + C\langle u,u\rangle, \quad \text{for all} \quad u \in \operatorname{dom}(\mathfrak{t}).$$

Recall also that $\mathcal{W}_j$, $j \in \mathcal{E}\cup\mathcal{I}$ denotes set of all functions $\psi_j \in \mathcal{H}_j$ which are absolutely continuous with square integrable derivative. According to (5) one sets

$$\mathcal{W} = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{W}_j.$$

LEMMA 1.12. *Under the Assumptions 1.1 and 1.4 the form $\delta_{\mathcal{M}}$ with $\mathcal{M} = \mathcal{M}(A,B)$ given in* (15) *is sectorial and closeable. Its closure $\overline{\delta_{\mathcal{M}}}$ is given by*

$$\overline{\delta_{\mathcal{M}}}[\psi] = \int_{\mathcal{G}} |\psi'|^2 - \langle LP^\perp\underline{\psi}, P^\perp\underline{\psi}\rangle_{\mathcal{K}}, \quad \psi \in \{\varphi \in \mathcal{W} \mid P\underline{\varphi} = 0\}$$

where P is the orthogonal projector onto $\operatorname{Ker} B$, $P^\perp = \mathbb{1} - P$ and L is computed from A, B by formula (18). *The operator $-\Delta(A,B)$ is associated with $\overline{\delta_{\mathcal{M}}}$ and the symmetric form $\operatorname{Re}\overline{\delta_{\mathcal{M}}}$ corresponds to the self–adjoint Laplace operator $-\Delta(A',B')$ with $A' = P + \operatorname{Re} L$ and $B' = P^\perp$.*

The proof of Lemma 1.12 uses the following elementary but important trace estimate, which is borrowed from [72].

LEMMA 1.13 (Trace estimate, [72, Lemma 8]). *Let $f \in \mathcal{W}_j \subset \mathcal{H}_j = L^2([0,a_j];\mathbb{C})$. Then*

$$|f(0)|^2 \leq \frac{2}{l}\|f\|^2_{\mathcal{H}_j} + l\|f'\|^2_{\mathcal{H}_j},$$

holds for any $0 < l \leq a_j$.

The statement of the lemma remains valid for $f \in \mathcal{W}_e \subset \mathcal{H}_e = L^2([0,\infty);\mathbb{C})$, $e \in \mathcal{E}$, with $0 < l < \infty$.

PROOF OF LEMMA 1.12. Inserting the representation (20) into the quadratic form $\delta_{\mathcal{M}}$ yields

$$\delta_{\mathcal{M}}[\psi] = \int_{\mathcal{G}} |\psi'|^2 - \langle LP^{\perp}\underline{\psi}, P^{\perp}\underline{\psi}\rangle_{\mathcal{K}}. \tag{21}$$

Obviously $\delta_{\mathcal{M}} \subset \overline{\delta_{\mathcal{M}}}$, and therefore one proves that $\overline{\delta_{\mathcal{M}}}$ is sectorial. Note that $\operatorname{Im}\overline{\delta_{\mathcal{M}}}[\psi] = -\langle \underline{\psi}, \operatorname{Im} L\underline{\psi}\rangle_{\mathcal{K}}$, and hence, since L as an operator in $\mathcal{K}$ is sectorial, there are $\gamma >$ and $C > 0$ such that

$$|\operatorname{Im}\langle \underline{\psi}, L\underline{\psi}\rangle_{\mathcal{K}}| \leq \gamma\langle \underline{\psi}, \operatorname{Re} L\underline{\psi}\rangle_{\mathcal{K}} + C\langle \underline{\psi}, \underline{\psi}\rangle_{\mathcal{K}}.$$

The trace estimate in Lemma 1.13 gives for sufficiently small $l > 0$ with $l \leq \min_{i\in\mathcal{I}} a_i$,

$$|\operatorname{Im}\langle \underline{\psi}, L\underline{\psi}\rangle_{\mathcal{K}}| \leq \gamma\langle \underline{\psi}, \operatorname{Re} L\underline{\psi}\rangle_{\mathcal{K}} + \frac{4C}{l}\|\psi\|^2_{\mathcal{H}} + 2Cl\|\psi'\|^2_{\mathcal{H}},$$

where the trace estimate has been applied to all endpoint of the edges. Choosing $l > 0$ small enough one can estimate the right hand side of the above inequality and one arrives at

$$|\operatorname{Im}\langle \underline{\psi}, L\underline{\psi}\rangle_{\mathcal{K}}| \leq \gamma \operatorname{Re}\overline{\delta}_{\mathcal{M}}[\psi] + \frac{4C}{l}\|\psi\|^2_{\mathcal{H}},$$

and hence $\delta_{\mathcal{M}}$ as well as $\overline{\delta_{\mathcal{M}}}$ are sectorial even in the larger domain $\mathcal{W}$. Note that the norm defined by $\left(\operatorname{Re}\overline{\delta_{\mathcal{M}}}[\psi] + C\|\psi\|^2_{\mathcal{H}}\right)^{1/2}$ is equivalent to the norm $\|\cdot\|_{\mathcal{W}}$ given by $\|\psi\|^2_{\mathcal{W}} = \|\psi\|^2_{\mathcal{H}} + \|\psi'\|^2_{\mathcal{H}}$, and that $\mathcal{W}_P = \{\psi \in \mathcal{W} \mid P\underline{\psi} = 0\}$ is a closed subspace of $\mathcal{W}$. Hence $\overline{\delta_{\mathcal{M}}}$ is a closed sectorial form. Note furthermore that the form $\overline{\delta_{\mathcal{M}}}$ is associated with the closed sectorial operator $-\Delta(A,B)$. Hence, for the uniqueness of the associated operator, compare for example [58, Theorem VI.2.1], the closure of $\delta_{\mathcal{M}}$ is indeed $\overline{\delta_{\mathcal{M}}}$.

Since $\overline{\delta_{\mathcal{M}}}$ is closed and sectorial the form $\operatorname{Re}\overline{\delta_{\mathcal{M}}}$ is closed and symmetric. Hence according to the first representation theorem, compare for example [58, Theorem VI.2.1], it corresponds to a self–adjoint operator. All forms of this type and the associated self–adjoint operators have been described in [72, Theorems 6 and 9]. Therefore, since

$$\operatorname{Re}\overline{\delta_{\mathcal{M}}}[\psi] = \int_{\mathcal{G}} |\psi'|^2 - \langle \operatorname{Re} LP^{\perp}\underline{\psi}, P^{\perp}\underline{\psi}\rangle_{\mathcal{K}}$$

the operator defined by $\operatorname{Re}\overline{\delta_{\mathcal{M}}}$ agrees with the Laplace operator $-\Delta(P + \operatorname{Re} L, P^{\perp})$. □

To prove the “only–if” part it is sufficient to show that assuming Assumption 1.1 and $QAP^{\perp} \neq 0$ gives that the numerical range of operator $-\Delta(A,B)$ contains the whole real line, and therefore it cannot be quasi–accretive.

LEMMA 1.14. *Let one of the Assumptions 1.1 and 1.4 be violated. Then $-\Delta(A,B)$ fails to be quasi–m–accretive.*

PROOF. Let Assumption 1.1 be violated. Then by Proposition 1.2 the operator $-\Delta(A,B)$ fails to be quasi–m–accretive. Therefore, suppose that Assumption 1.1 holds and Assumption 1.4 is violated.

Consider for simplicity the parametrisation (17) instead of the parametrisation (16). Inserting the boundary condition (17) into the quadratic form (15) yields

$$\delta_{\mathcal{M}}[\psi] = \int_{\mathcal{G}} |\psi'|^2 - \langle P^{\perp}\underline{\psi}, P^{\perp}A'\underline{\psi}\rangle_{\mathcal{K}} + \langle P\underline{\psi}, P\underline{\psi}'\rangle_{\mathcal{K}},$$

where $\mathcal{M}(A,B) = \mathcal{M}(A',B')$ and P is the orthogonal projector onto $\operatorname{Ker} B'$. Since QA is surjective by Assumption 1.1 also PA' is surjective, and one has

$$\dim \operatorname{Ker} PA' = \dim \operatorname{Ran} P^{\perp}.$$

Therefore $QAP^{\perp} \neq 0$ implies $PA'P^{\perp} \neq 0$ which delivers $\operatorname{Ker} PA' \neq \operatorname{Ran} P^{\perp}$. This in turn implies that there is a vector α such that

$$PA'\alpha = 0, \quad \text{but} \quad P\alpha \neq 0. \tag{22}$$

Using this vector one constructs explicitly a sequence $u_n \in \operatorname{Dom}(-\Delta(A',B'))$, $n \in \mathbb{N}$, such that $\operatorname{Re}\langle u_n, -\Delta(A',B')u_n\rangle \to -\infty$, for $n \to \infty$.

For simplicity suppose first that $\mathcal{G}$ is a finite star graph, that is $\mathcal{I} = \emptyset$ and $|\mathcal{E}| = m$.

First one defines an auxiliary matrix-valued function on the half-line. Let $0 < a < b < c$ be positive numbers, $H \in \operatorname{End}(\mathcal{K})$ an arbitrary matrix and $p(H;x)$ and $q(H;x)$ functions in x and H. One defines

$$\Phi_H[p,q;a,b,c]\colon [0,\infty) \to \operatorname{End}(\mathcal{K}),$$

by

$$\Phi_H[p,q;a,b,c](x) = \begin{cases} e^{Hx}, & x \in [0,a], \\ p(H;x), & x \in (a,b), \\ q(H;x), & x \in [b,c), \\ 0, & x \in [c,\infty). \end{cases}$$

Consider for $n \geq 1$ the sequence of matrices

$$H_n = -\begin{pmatrix} P^{\perp}A'P^{\perp} & P^{\perp}A'P \\ 0 & nP \end{pmatrix}$$

and note that

$$2\operatorname{Re} H_n = \begin{pmatrix} 2\operatorname{Re} P^{\perp}A'P^{\perp} & P^{\perp}A'P \\ (P^{\perp}A'P)^* & 2nP \end{pmatrix}$$

and that

$$2\operatorname{Im} H_n = \begin{pmatrix} 2\operatorname{Im} P^{\perp}A'P^{\perp} & P^{\perp}A'P \\ -(P^{\perp}A'P)^* & 0 \end{pmatrix}.$$

In order to analyse these bounded block operator matrices the concept of the quadratic numerical range is helpful, for further information on this topic see the book [88] and the references therein. As the numerical ranges of the diagonal blocks are contained in the numerical range of the whole block operator matrix one obtains that $\|\operatorname{Re} H_n\| \sim n$ for large n. Therefore also

$$\|H_n\| \leq \left(\|\operatorname{Re} H_n\|^2 + \|\operatorname{Im} H_n\|^2\right)^{1/2} \sim n \qquad \text{for } n \text{ large.}$$

Define now for sequences $(a_n), (b_n), (c_n)$ with $0 < a_n < b_n < c_n$ for $n \geq 1$ the polynomial $p_n(H_n;\cdot)$ in x by

$$p_n(H_n;x) = \beta_n \frac{(x-b_n)^{n+1}}{n+1} + \gamma_n$$

with coefficients

$$\beta_n = \frac{H_n e^{H_n a_n}}{(a_n - b_n)^n} \quad \text{and} \quad \gamma_n = \left[\mathbb{1} - \frac{(a_n - b_n)}{n+1} H_n\right] e^{H_n a_n}.$$

This assures that

$$\begin{aligned} p_n(H_n;a_n) &= e^{Ha_n}, & \tfrac{d}{dx} p_n(H_n;a_n) &= H_n e^{H_n a_n}, \\ p_n(H_n;b_n) &= \gamma_n \quad \text{and} & \tfrac{d}{dx} p_n(H_n;b_n) &= 0. \end{aligned}$$

Furthermore choose q_n to be a polynomial in x such that

$$\begin{aligned} q_n(H_n;b_n) &= \gamma_n, & \tfrac{d}{dx} q_n(H_n;b_n) &= 0, \\ q_n(H_n;c_n) &= 0 \quad \text{and} & \tfrac{d}{dx} q_n(H_n;c_n) &= 0 \end{aligned}$$

hold for all $n \geq 1$. This gives that the function $\Phi_{H_n}[p_n, q_n; a_n, b_n, c_n]$ is a function in the Sobolev space $H^2([0,\infty), \mathrm{End}(\mathcal{K}))$ for all $n \in \mathbb{N}$, and by construction it is even compactly supported.

Now with the vector α chosen above, compare (22), one sets

$$\{u_n\}_e(x) := \left\{\Phi_{H_n}[p_n, q_n; a_n, b_n, c_n](x)\alpha\right\}_e, \quad \text{for } e \in \mathcal{E}.$$

This defines functions $u_n \colon \mathcal{G} \to \mathbb{C}$ for $n \in \mathbb{N}$. By construction one has $u_n \in \mathcal{D}$. One proves now that $u_n \in \operatorname{Dom}(-\Delta(A',B'))$. Indeed,

$$\Phi_{H_n}[p_n, q_n; a_n, b_n, c_n](0)\alpha = \alpha \quad \text{and} \quad \frac{d}{dx} \Phi_{H_n}[p_n, q_n; a_n, b_n, c_n](\cdot)\alpha\Big|_{x=0} = H_n \alpha.$$

Therefore

$$\underline{u_n} = \begin{pmatrix} P^\perp \alpha \\ P\alpha \end{pmatrix} \quad \text{and} \quad \underline{u_n}' = -\begin{pmatrix} P^\perp A' P^\perp & P^\perp A' P \\ 0 & nP \end{pmatrix} \begin{pmatrix} P^\perp \alpha \\ P\alpha \end{pmatrix}$$

for all $n \in \mathbb{N}$. From $\underline{u_n} = \alpha$, $\begin{pmatrix} PA'P^\perp & PA'P \end{pmatrix} \alpha = 0$ and (22) it follows that

$$A'\underline{u_n} + B'\underline{u_n}' = \begin{pmatrix} P^\perp A' P^\perp & P^\perp A' P \\ PA'P^\perp & PA'P \end{pmatrix} \begin{pmatrix} P^\perp \underline{u_n} \\ P\underline{u_n} \end{pmatrix} + \begin{pmatrix} P^\perp & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} P^\perp \underline{u_n}' \\ P\underline{u_n}' \end{pmatrix} = 0.$$

This implies that $u_n \in \operatorname{Dom}(-\Delta(A',B'))$ for all $n \in \mathbb{N}$. Inserting u_n into the quadratic form (15) gives

$$\begin{aligned} \langle u_n, -\Delta(A',B') u_n \rangle &= \int_{\mathcal{G}} |u_n'|^2 + \langle \underline{u_n}, \underline{u_n}' \rangle_{\mathcal{K}} \\ &= \int_{\mathcal{G}} |u_n'|^2 - \langle P^\perp \alpha, P^\perp A' \alpha \rangle_{\mathcal{K}} - n \langle P\alpha, P\alpha \rangle_{\mathcal{K}}. \end{aligned}$$

The term $-\langle P^\perp \alpha, P^\perp A' \alpha \rangle_{\mathcal{K}}$ is bounded. Chose now

$$a_n = \frac{e^{-2\|H_n\|}}{\|H_n\|^2}, \quad b_n = 2\frac{e^{-2\|H_n\|}}{\|H_n\|^2} \quad \text{and } c_n = \text{constant},$$

for n sufficiently large. With this one obtains

$$\begin{aligned}\int_{a_n}^{b_n} \left|\tfrac{d}{dx}(p_n)(H_n;x)\alpha\right|^2 dx &\leq m\frac{\|H_n\|^2}{|b_n-a_n|^{2n}}\|e^{H_n}\|^2\|\alpha\|^2\int_{a_n}^{b_n}|x-b_n|^{2n}dx\\ &\leq m\frac{\|H_n\|^2 e^{2\|H_n\|}\|\alpha\|^2}{(2n+1)}|a_n-b_n| \to 0, \quad \text{for } n\to\infty,\end{aligned}$$

where $m=|\mathcal{E}|$. Furthermore one has

$$\begin{aligned}\int_0^{a_n}|H_n e^{H_n x}\alpha|^2 dx &\leq m\|\alpha\|^2\|H_n\|^2\int_0^{a_n} e^{2\|H_n\|x}dx\\ &= \frac{m}{2}\|\alpha\|^2\|H_n\|\left(e^{2\|H_n\|a_n}-1\right)\to 0, \quad \text{for } n\to\infty.\end{aligned}$$

Since $\|\gamma_n\|\to 1$ for $n\to\infty$ and $\frac{d}{dx}p_n(H;b_n)=0$, there exist constants $C,c>0$ such that

$$c \leq \int_{b_n}^{c} |\tfrac{d}{dx}(q_n(H_n;x))\alpha|^2 dx \leq C \tag{23}$$

holds for all $n\in\mathbb{N}$. Together this gives that $\int_{\mathcal{G}}|u_n'|^2$ is uniformly bounded whereas $\operatorname{Re}\langle \underline{u_n}, \underline{u_n}'\rangle \to -\infty$ and therefore

$$\operatorname{Re}\langle u_n, -\Delta(A',B')u_n\rangle \to -\infty, \quad \text{for } n\to\infty.$$

Now one estimates the L^2–norm of u_n. Since $u_n\in H^2([0,c_n],\operatorname{End}(\mathcal{K}))$, $u_n(c_n)=0$ and $c_n=$ constant for n sufficiently large it follows that a Poincaré inequality can be applied to u_n and hence there is a constant $C>0$ which is uniform in n such that

$$\int_{\mathcal{G}}|u_n|^2 \leq C\int_{\mathcal{G}}|u_n'|^2 \quad \text{for all } n\in\mathbb{N}.$$

At the same time one has that

$$0 < \int_{b_n}^{c_n}|q_n(H_n;x)\alpha|^2 < \int_{\mathcal{G}}|u_n|^2 \quad \text{for all } n\in\mathbb{N}.$$

Hence $\|u_n\|$ is uniformly bounded from below and from above. Consequently the operator $-\Delta(A,B)=-\Delta(A',B')$ is not quasi–accretive. This proves Lemma 1.14 for the case of star graphs.

Note that, the construction of $\Phi_{H_n}[p_n,q_n;a_n,b_n,c_n](\cdot)$ has been done only for simplicity on the half line. Actually only the locality of the boundary conditions is needed. Locality of the boundary conditions can be achieved always by collapsing all vertices into one single vertex. This method of "localisation" has been used frequently in the literature, for example recently in [29]. So, having a Laplacian $-\Delta(A,B)$ on a metric graph $(\mathcal{G},\underline{a})$ with $\mathcal{G}=(V,\mathcal{I},\mathcal{E},\partial)$ one considers instead $(\mathcal{G}',\underline{a})$ with $\mathcal{G}=(\{v\},\mathcal{I},\mathcal{E},\partial')$, where $\partial(e)=v$ and $\partial(i)=(v,v)$ for all $i\in\mathcal{I}$ and $e\in\mathcal{E}$. Since neither the edges nor the space of boundary values are changing one can define again the operator $-\Delta(A,B)$ on this auxiliary graph, and it is equivalent to the initial operator differing from it only formally. On this graph one can consider $\Phi_{H_n}[p_n,q_n;a_n,b_n,c_n](\cdot)$ for c_n small enough, that is $c_n<a_i$ for all $i\in\mathcal{I}$. Restricting the functions u_n to small neighbourhoods of the vertex carries the proof over to arbitrary finite metric graphs with internal edges. $\square$

PROOF OF THEOREM 1.6. If both Assumptions 1.1 and 1.4 are satisfied then by Proposition 1.2 and Lemma 1.12 it follows that $-\Delta(A, B)$, where $\mathcal{M} = \mathcal{M}(A, B)$, is quasi–m–accretive and therefore even m–sectorial. The statement on the form corresponding to $-\Delta(A, B)$ and the statement on the real part follow immediately from Lemma 1.13. If one of the assumptions is violated it follows from Lemma 1.14 that $-\Delta(A, B)$ fails to be quasi–m–accretive. □

REMARK 1.15. *Let A, B satisfy both Assumptions 1.1 and 1.4. Then in the quadratic form associated with $-\Delta(A, B)$ the traces $\underline{\psi}'$ cancel out and only boundary values involving $\underline{\psi}$ remain. It follows from the trace estimate in Lemma 1.13 that the map $\psi \to \underline{\psi}$ is bounded as a map between the Hilbert spaces $\mathcal{W}$ and $\mathcal{K}$, and consequently one is able to prove that $-\Delta(A, B)$ is m–sectorial. Assuming only Assumption 1.1 one observes that the traces $\underline{\psi}'$ do not cancel out in the corresponding quadratic form and the evaluation of the derivatives at the vertices is not controlled by other boundary conditions. The proof of Lemma 1.14 takes advantage of the fact that the map $\psi \to \underline{\psi}'$ is not bounded in the norm of the Hilbert space $\mathcal{W}$. This makes Example 1.9 representative for the boundary conditions that satisfy both Assumptions 1.1 and 1.4. Example 1.11 is typical for the boundary conditions that satisfy only Assumption 1.1, particularly in the case $\tau = 0$.*

PROOF OF THEOREM 1.7. In [12, Theorem 1] it is stated that a self–adjoint Laplace operator $-\Delta(A_{sa}, B_{sa})$ is non-negative if and only if

$$A_{sa}B_{sa}^* + B_{sa}M_0(\underline{a})B_{sa}^* \leq 0,$$

where $M_0(\underline{a})$ is the matrix given in Theorem 1.7, compare also Proposition 2.1 and Remark 2.2 in Chapter 2. Therefore the operator $-\Delta(A, B)$ is m–accretive if and only if the Assumptions 1.1 and 1.4 are satisfied and the form $\operatorname{Re} \overline{\delta_{\mathcal{M}}}$ is non-negative. According to Lemma 1.13 this is the case if and only if $-\Delta(A', B') \geq 0$ with $A' = P + \operatorname{Re} L$ and $B' = P^{\perp}$. Using the cited result this is equivalent to the condition

$$\operatorname{Re} AB^* + BM_0(\underline{a})B^* \leq 0.$$

It remains to show that $\operatorname{Re} AB^* + BM_0(\underline{a})B^* \leq 0$ implies that Assumption 1.4 holds. Let Assumption 1.1 be satisfied. Then one can assume without loss of generality $B = P^{\perp}$. The decomposition of A with respect to P and $P^{\perp}$ gives

$$AB^* = \begin{pmatrix} P^{\perp}AP^{\perp} & P^{\perp}AP \\ PAP^{\perp} & PAP \end{pmatrix} \begin{pmatrix} P^{\perp} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} P^{\perp}AP^{\perp} & 0 \\ PAP^{\perp} & 0 \end{pmatrix}$$

and, hence,

$$\operatorname{Re}(AB^*) = \frac{1}{2} \begin{pmatrix} 2\operatorname{Re}(P^{\perp}AP^{\perp}) & (PAP^{\perp})^* \\ PAP^{\perp} & 0 \end{pmatrix}$$

and

$$BM_0(\underline{a})B^* = \begin{pmatrix} P^{\perp}M_0(\underline{a})P^{\perp} & 0 \\ 0 & 0 \end{pmatrix}.$$

The numerical range of such block-matrix operators is discussed in the following elementary lemma. It covers a particular case of the problem of the positive completion of diagonal block-operator matrices, see [48] and the references therein, where the general problem is discussed.

LEMMA 1.16. *Let M be a bounded self–adjoint block operator matrix of the form*

$$M = \begin{bmatrix} A & B^* \\ B & 0 \end{bmatrix}, \quad \textit{where} \quad A = A^*.$$

Then $M \leq 0$ ($M \geq 0$) if and only if $A \leq 0$ ($A \geq 0$) and $B \equiv 0$.

The proof of this lemma makes implicitly use of the concept of the quadratic numerical range. For further references on this topic I highly recommend the book [88].

Applying Lemma 1.16 to the boundary conditions defined by A, B gives that

$$\mathrm{Re}\,(AB^*) + BM_0(\underline{a})B^* \leq 0 \quad \text{if and only if} \quad PAP^\perp \equiv 0,$$

which is nothing but Assumption 1.4. □

PROOF OF LEMMA 1.16. The numerical range of A is included in the numerical range of M therefore a necessary condition for M to be negative definite is that A is negative definite. Assume now that $B \neq 0$. Then there exists u and v such that $b = \langle Bu, v\rangle \neq 0$. Consider the 2×2–matrix

$$M(u,v) = \begin{bmatrix} \langle Au, u\rangle & \langle Bu, v\rangle \\ \langle B^*v, u\rangle & 0 \end{bmatrix} = \begin{bmatrix} a & b \\ b^* & 0 \end{bmatrix}$$

with $a = \langle Au, u\rangle$, which has the two eigenvalues

$$\lambda_+ = \frac{1}{2}a + \frac{1}{2}\sqrt{a^2 + 4|b|^2} \quad \text{and} \quad \lambda_- = \frac{1}{2}a - \frac{1}{2}\sqrt{a^2 + 4|b|^2}.$$

The number λ_- is negative whereas λ_+ is positive and hence the numerical range of M takes positive as well as negative values. The endpoints of the numerical range are in the spectrum of the self–adjoint operator M, compare [46, Theorem 1.5-5, Corollary 1.5-6], which means that M is indefinite. Assuming the other way around that $A \leq 0$ and $B \equiv 0$ the statement follows. For $M \geq 0$ the proof is analogous. □

CHAPTER 2

The negative spectrum of self–adjoint Laplace operators

This chapter deals with the negative spectrum of self–adjoint Laplace operators on finite metric graphs. In the article [72] P. Kuchment proved that on a finite not necessarily compact, metric graph all self–adjoint Laplacians are semi–bounded from below and furthermore the negative spectrum is purely discrete. P. Kuchment, see [72, Corollary 10] and V. Kostrykin together with R. Schrader, see [63, Theorem 3.10] gave two different lower bounds on the bottom of the spectrum of self–adjoint Laplacians on finite metric graphs. The exercise discussed here is to give for each negative eigenvalue of a self–adjoint Laplacian estimates from below and from above. In the previous chapter it has been proven that the real part of a quasi–m–accretive Laplacian on a metric graph is a certain self–adjoint Laplacian. The smallest eigenvalue of this self–adjoint Laplace operator is exactly the growth bound of the semigroup generated by the quasi–m–accretive operator, compare Remark 1.8 in Chapter 1. Therefore, lower and upper bounds on the negative spectrum give a priori estimates on the growth bound of the corresponding semigroup.

The problem of calculating the number of negative eigenvalues has been solved by A. Luger and J. Behrndt in [12], where variational principles for self–adjoint operator pencils, see [34] were used. In the present study estimates on the negative eigenvalues from above and from below are derived applying the same variational methods to the eigenvalues themselves rather than to their number. Three types of estimates are obtained, each is optimal in a certain situation. In particular, the previously known lower bounds on the spectrum from the works [72] and [63] are re–obtained.

The chapter is structured as follows: first the negative eigenvalues of self-adjoint Laplacians on metric graphs are discussed. This is followed by the main results, the estimates on the negative eigenvalues. Thereafter the eigenvalue zero of a self–adjoint Laplacian defined on a compact metric graph is discussed and Poincaré type inequalities on compact metric graphs are obtained. Finally, in Section 2.4 the variational methods are presented and used to prove the bounds on the negative eigenvalues stated in Section 2.2. Parts of this chapter are published in the article [53].

2.1. Negative eigenvalues

Let be given a finite metric graph $(\mathcal{G}, \underline{a})$. One sets

$$a_{\min} := \min_{i\in\mathcal{I}} a_i \quad \text{and} \quad a_{\max} := \max_{i\in\mathcal{I}} a_i.$$

As already remarked self–adjoint extensions of $-\Delta^0$ can be discussed in terms of boundary conditions. Let A and B be linear maps in $\mathcal{K}$. Recall that $(A,\, B)$ denotes the linear map from $\mathcal{K}^2 = \mathcal{K} \oplus \mathcal{K}$ to $\mathcal{K}$ defined by

$$(A,\, B)(\chi_1 \oplus \chi_2) = A\chi_1 + B\chi_2,$$

for $\chi_1, \chi_2 \in \mathcal{K}$, and one sets

$$\mathcal{M}(A, B) = \operatorname{Ker}(A,\, B). \tag{24}$$

With any subspace $\mathcal{M} \subset \mathcal{K}^2$ of the form (24) one can associate an extension $-\Delta(\mathcal{M})$ of $-\Delta^0$ which acts as $-\Delta$ on the domain

$$\operatorname{Dom}(-\Delta(\mathcal{M})) = \{\psi \in \mathcal{D} \mid [\psi] \in \mathcal{M}\}.$$

An equivalent description is that $\operatorname{Dom}(-\Delta(\mathcal{M}))$ consists of all functions $\psi \in \mathcal{D}$ that satisfy the linear boundary conditions

$$A\underline{\psi} + B\underline{\psi}' = 0.$$

With A and B as in (24) one also writes

$$-\Delta(\mathcal{M}) = -\Delta(A, B).$$

All self-adjoint extensions of $-\Delta^0$ can be parametrized by matrices $A, B \in \operatorname{End}(\mathcal{K})$, which have the following two properties:

(1) $(A,\, B)\colon \mathcal{K}^2 \to \mathcal{K}$ is surjective and
(2) AB^* self-adjoint,

see for example [60, 62] or [47] and the discussions therein. The choice of matrices A and B is not unique, in the sense that two different parametrizations by maps $(A,\, B)$ and $(A',\, B')$ describe the same operator if and only if the Lagrangian subspaces $\mathcal{M}(A, B)$ and $\mathcal{M}(A', B')$ agree. In [72, Corollary 5] a unique way to parametrize a self–adjoint Laplacian in terms of an orthogonal projection P acting in $\mathcal{K}$ and a Hermitian operator L acting in $\operatorname{Ran} P^{\perp} \subset \mathcal{K}$ is proposed. For any self–adjoint Laplacian $-\Delta(A, B)$ there are unique such P and L, such that $-\Delta(A, B) = -\Delta(A', B')$ holds with $A' = L + P$ and $B' = P^{\perp}$. The change over is given by

$$L = \left(B\,|_{\operatorname{Ran} B^*}\right)^{-1} AP^{\perp}, \tag{25}$$

where P denotes the orthogonal projector onto $\operatorname{Ker} B \subset \mathcal{K}$ and $P^{\perp} = \mathbb{1} - P$ is the complementary projector. The strictly positive part of the operator L is denoted by L_+, its strictly negative part by L_- and the orthogonal projector onto the kernel of L, considered as a map in the Hilbert space $\operatorname{Ran} P^{\perp} = \operatorname{Ker} P$, is denoted by L_0.

For a self-adjoint Laplace operator $-\Delta(A, B)$ on a finite metric graph one has $\sigma_{ess}(-\Delta(A, B)) \subset [0, \infty)$ and the negative spectrum of $-\Delta(A, B)$ consists, at the most, of only finitely many eigenvalues of finite multiplicity since the minimal operator $-\Delta^0$ has only finite deficiency indices. A fundamental system of the equation

$$\left(-\frac{d^2}{dx^2} + \kappa^2\right) u(\cdot, \kappa) = 0, \qquad \kappa \neq 0$$

is $e^{-\kappa x}, e^{\kappa x}$. For $\kappa > 0$ only the first mentioned function $e^{-\kappa x}$ is square integrable on the half line $[0, \infty)$ and hence on the external edges. Consequently an *Ansatz* for a square integrable eigenfunction to a negative eigenvalue $-\kappa^2$ is

$$\psi(x, i\kappa) = \begin{cases} s_j(i\kappa) e^{-\kappa x_j}, & j \in \mathcal{E}, \\ \alpha_j(i\kappa) e^{-\kappa x_j} + \beta_j(i\kappa) e^{\kappa x_j}, & j \in \mathcal{I}. \end{cases}$$

The function $\psi(\cdot, i\kappa)$ has the traces

$$\underline{\psi(\cdot, i\kappa)} = X\,(i\kappa, \underline{a}) \begin{bmatrix} \{s_j(i\kappa)\}_{j\in\mathcal{E}} \\ \{\alpha_j(i\kappa)\}_{j\in\mathcal{I}} \\ \{\beta_j(i\kappa)\}_{j\in\mathcal{I}} \end{bmatrix}, \qquad \underline{\psi(\cdot, i\kappa)'} = -\kappa\cdot Y\,(i\kappa, \underline{a}) \begin{bmatrix} \{s_j(i\kappa)\}_{j\in\mathcal{E}} \\ \{\alpha_j(i\kappa)\}_{j\in\mathcal{I}} \\ \{\beta_j(i\kappa)\}_{j\in\mathcal{I}} \end{bmatrix},$$

where

$$X\,(i\kappa, \underline{a}) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & \mathbb{1} \\ 0 & e^{-\kappa\underline{a}} & e^{\kappa\underline{a}} \end{bmatrix} \quad\text{and}\quad Y\,(i\kappa, \underline{a}) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & -\mathbb{1} \\ 0 & -e^{-\kappa\underline{a}} & e^{\kappa\underline{a}} \end{bmatrix}$$

are given with respect to the decomposition $\mathcal{K} = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^{-} \oplus \mathcal{K}_{\mathcal{I}}^{+}$ given in (12). The function $\psi(\cdot, i\kappa)$ is indeed an eigenfunction to the eigenvalue $-\kappa^2 < 0$ if and only if $\psi(\cdot, i\kappa) \in \operatorname{Dom}(-\Delta(A,B))$, where $\kappa > 0$ is the positive square root of κ^2. This is the case if and only if the *Ansatz* function $\psi(\cdot, i\kappa)$ satisfies the boundary conditions, which are encoded in the equation

$$Z\,(i\kappa, \underline{a}, A, B) \begin{bmatrix} \{s_j(i\kappa)\}_{j\in\mathcal{E}} \\ \{\alpha_j(i\kappa)\}_{j\in\mathcal{I}} \\ \{\beta_j(i\kappa)\}_{j\in\mathcal{I}} \end{bmatrix} = 0, \tag{26}$$

where

$$Z\,(i\kappa, \underline{a}, A, B) = AX(i\kappa, \underline{a}) - \kappa\, BY(i\kappa, \underline{a}).$$

The matrices $X\,(i\kappa, \underline{a})$ and $Y\,(i\kappa, \underline{a})$ are invertible for $\kappa > 0$. Hence equation (26) has non–trivial solutions if and only if

$$\det(A + BM(\kappa, \underline{a})) = 0 \quad\text{with}\quad M(\kappa, \underline{a}) = -\kappa\cdot Y(i\kappa, \underline{a})X(i\kappa, \underline{a})^{-1}. \tag{27}$$

The operator $M(\kappa, \underline{a})$ has the diagonalisation

$$M\,(\kappa, \underline{a}) = QD\,(\kappa, \underline{a})\,Q$$

with

$$Q = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \frac{\mathbb{1}}{\sqrt{2}} & \frac{\mathbb{1}}{\sqrt{2}} \\ 0 & \frac{\mathbb{1}}{\sqrt{2}} & -\frac{\mathbb{1}}{\sqrt{2}} \end{bmatrix} \quad\text{and}\quad D(\kappa, \underline{a}) = \begin{bmatrix} -\kappa & 0 & 0 \\ 0 & \lambda\,(\kappa, \underline{a}) & 0 \\ 0 & 0 & \mu\,(\kappa, \underline{a}) \end{bmatrix},$$

where

$$\lambda\,(\kappa, \underline{a}) = -\kappa\tanh(\kappa\underline{a}/2) \quad\text{and}\quad \mu\,(\kappa, \underline{a}) = \frac{-\kappa}{\tanh(\kappa\underline{a}/2)}$$

are $|\mathcal{I}|\times|\mathcal{I}|$–diagonal matrix with entries

$$\{\lambda\,(\kappa, \underline{a})\}_{i,j\in\mathcal{I}} = -\delta_{ij}\kappa\tanh(\kappa a_i/2) \quad\text{and}\quad \{\mu\,(\kappa, \underline{a})\}_{i,j\in\mathcal{I}} = \delta_{ij}\frac{-\kappa}{\tanh(\kappa a_i/2)}.$$

Note that the unitary operator Q satisfies even $Q^2 = \mathbb{1}$ and $Q^* = Q$. One sets

$$M(0, \underline{a}) := \lim_{\kappa\to 0} M(\kappa, \underline{a}), \quad\text{hence}\quad M(0, \underline{a}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -\frac{1}{\underline{a}} & \frac{1}{\underline{a}} \\ 0 & \frac{1}{\underline{a}} & -\frac{1}{\underline{a}} \end{bmatrix}, \tag{28}$$

because

$$\lim_{\kappa\to 0} -\kappa\tanh(\kappa a_i/2) = 0 \quad \text{and} \quad \lim_{\kappa\to 0} \frac{-\kappa}{\tanh(\kappa\, a_i/2)} = -\frac{2}{a_i}.$$

One concludes that $M(0,\underline{a})$ has the eigenvalues 0 and $-\frac{2}{a_i}$, $i\in\mathcal{I}$, and consequently $M(0,\underline{a})\leq 0$. Note that $M(0,\underline{a}) = M_0(\underline{a})$, where $M_0(\underline{a})$ is defined in Theorem 1.7 in Chapter 1.

Consider instead of A, B the equivalent boundary conditions A', B', where $A' = L + P$ and $B' = P^{\perp}$ with P the orthogonal projector onto $\operatorname{Ker} B$ and L a Hermitian operator in $\operatorname{Ran} P^{\perp}$. The orthogonal decomposition

$$\mathcal{K} = (\operatorname{Ran} P) \oplus (\operatorname{Ran} P^{\perp})$$

induces in (27) the block structure

$$\det\left(\begin{bmatrix} P^{\perp}LP^{\perp} & 0 \\ 0 & P\end{bmatrix} + \begin{bmatrix} P^{\perp}M(\kappa,\underline{a})P^{\perp} & P^{\perp}M(\kappa,\underline{a})P \\ 0 & 0\end{bmatrix}\right) = 0.$$

Consequently $-\kappa^2$ is a negative eigenvalue of $-\Delta(A,B)$ if and only if the Hermitian operator

$$L(\kappa,\underline{a}) := \left(L + P^{\perp}M(\kappa,\underline{a})P^{\perp}\right), \quad \kappa > 0,$$

considered as an operator in the Hilbert space $\operatorname{Ran} P^{\perp}$ is not invertible. The multiplicity of $-\kappa^2$ equals the dimension of $\operatorname{Ker} L(\kappa,\underline{a})$. One sets $L(0,\underline{a}) = L + P^{\perp}M(0,\underline{a})P^{\perp}$. On star graphs, that is for $\mathcal{I}=\emptyset$, one has simply $L(\kappa) = L - \kappa P^{\perp}$.

Note that by the use of $L(\cdot,\underline{a})$ instead of $Z(\cdot,A,B,\underline{a})$ the problem of solving the eigenvalue equation transforms to a non–linear eigenvalue problem with values in the set of the Hermitian operators. Thus, variational methods apply to $L(k,\underline{a})$, and since the function $L(\cdot,\underline{a})$ is strictly decreasing and continuous one can also apply variational methods to the generalized eigenvalue problem associated with $L(\cdot,\underline{a})$. This has been used to determine the number of negative eigenvalues in [12, Theorem 1], which is reformulated here as

PROPOSITION 2.1 ([12, Theorem 1]). *The number of negative eigenvalues of the self–adjoint Laplace operator $-\Delta(A,B)$ (counted with multiplicities) is given by the number of positive eigenvalues of $L(0,\underline{a})$ (counted with multiplicities). In particular, $-\Delta(A,B)$ is non–negative if and only if the operator $L(0,\underline{a})$ is non–positive.*

REMARK 2.2. *Let $-\Delta(A,B)$ be self–adjoint, P be the orthogonal projector onto $\operatorname{Ker} B$ and let L be given by (25). Then the operator $L(\kappa,\underline{a}) = \left(L + P^{\perp}M(\kappa,\underline{a})P^{\perp}\right)$ as an operator in the space $\operatorname{Ran} P^{\perp}$ is invertible if and only if the operator*

$$\tau_{A,B}(\kappa,\underline{a}) = AB^* + BM(\kappa,\underline{a})B^*$$

considered as an operator in the space $\operatorname{Ran} B$ is invertible. In the original formulation of [12, Theorem 1] the operator $\tau_{A,B}(0,\underline{a})$ is used instead of $L(0,\underline{a})$. The vectors of boundary values $\underline{\Psi}$ and $\underline{\Psi}'$ used in the article [12] differ only by a permutation from the vectors $\underline{\psi}$ and $\underline{\psi}'$ used here. In the original formulation of [12, Theorem 1] the operator $\tau_{A,B}(0,\underline{a})$, up to this permutation, is used instead of $L(0,\underline{a})$.

2.2. Bounds on the negative eigenvalues

Applying the above mentioned variational methods used in the article [12] delivers three different lower and upper bounds on each of the negative eigenvalues of a self–adjoint Laplacian $-\Delta(A,B)$. Each type of bound reflects the decay properties of one of the three blocks of the diagonal block operator matrix $D(\kappa,\underline{a})$. The estimates are obtained by proposing matrix valued functions, which are majorants or minorants to the function $L(\cdot,\underline{a})$ in the sense of quadratic forms.

Denote by

$$-\kappa_1^2 \leq \ldots \leq -\kappa_n^2 < 0$$

the negative eigenvalues of $-\Delta(A,B)$ (counted with multiplicities). For technical reasons it is convenient to consider the positive square roots of the absolute value of the negative eigenvalues, which are

$$\kappa_1 \geq \ldots \geq \kappa_n > 0$$

(counted with multiplicities). By Proposition 2.1 the number of negative eigenvalues of the operator $-\Delta(A,B)$ and the number of positive eigenvalues of $L(0,\underline{a})$ coincide. The positive eigenvalues of $L(0,\underline{a})$ are

$$l_1 \geq \ldots \geq l_n > 0$$

(counted with multiplicities) and $l_1 = \|L_+(0,\underline{a})\|$, where $L_+(0,\underline{a})$ denotes the positive part of $L(0,\underline{a})$. For fixed $l>0$ and $a>0$ the equation

$$l = \frac{\kappa}{\tanh(\kappa a/2)} - \frac{2}{a}$$

has a unique positive solution, which is denoted by $\eta(l,a)$. Consequently, for $l > \frac{2}{a}$ the equation

$$l = \frac{\kappa}{\tanh(\kappa a/2)}$$

has the unique positive solution $\eta(l-\frac{2}{a},a)$. For $l>0$ fixed and $a_{\min} < a_{\max}$ one has $\eta(l,a_{\max}) < \eta(l,a_{\min})$ which follows from the forthcoming inequality (31).

THEOREM 2.3. *Let $-\Delta(A,B)$ be self–adjoint. Then the square roots of the absolute values of the negative eigenvalues of $-\Delta(A,B)$ obey the two–sided estimates*

$$l_i \leq \kappa_i \leq \eta(l_i, a_{\min}), \quad 1 \leq i \leq n.$$

The lower bound on the spectrum

$$-\eta(l_1,a_{\min})^2 \leq -\Delta(A,B)$$

is optimal – that is the number $-\eta(l_1,a_{\min})^2$ is indeed an eigenvalue – if and only if

$$\mathit{span}\left\{ \begin{bmatrix} 0 \\ e_i \\ -e_i \end{bmatrix} \middle| a_i = a_{\min} \right\} \cap \operatorname{Ker}(L(0,\underline{a}) - l_1) \neq \{0\},$$

where e_i denotes the i–th canonical basis vector in $\mathcal{K}_{\mathcal{I}}^+$ and $\mathcal{K}_{\mathcal{I}}^-$, respectively, and $l_1 = \|L_+(0,\underline{a})\|$ is the largest positive eigenvalue of $L(0,\underline{a})$.

The proof of the above theorem is based on certain estimates on the operator valued function $L(\cdot, \underline{a})$. Other types of estimates on $L(\cdot, \underline{a})$ deliver similar theorems. The proofs are given in the next but one section along with a discussion of the variational methods used.

There are at least n positive eigenvalues of L (counted with multiplicities) because $L \geq L(0, \underline{a})$. Denote by

$$m_1 \geq \ldots \geq m_n > 0$$

the n largest positive eigenvalues of L (counted with multiplicities) and note that $m_1 = \|L_+\|$. For $m > 0$ the equation

$$m = \kappa \tanh(\kappa a/2)$$

has a unique positive solution $\nu(m, a)$. Furthermore for $m > \frac{2}{a}$ the equation

$$m = \frac{\kappa}{\tanh(\kappa a/2)}$$

has the unique positive solution $\eta(m - \frac{2}{a}, a)$.

THEOREM 2.4. *Let $-\Delta(A, B)$ be self–adjoint. Then the square roots of the absolute values of the negative eigenvalues of $-\Delta(A, B)$ obey the estimate*

$$0 < \kappa_i \leq \nu(m_i, a_{\min}), \quad 1 \leq i \leq n.$$

The lower bound on the spectrum

$$-\nu(m_1, a_{\min})^2 \leq -\Delta(A, B)$$

is optimal – that is the number $-\nu(m_1, a_{\min})^2$ is indeed an eigenvalue – if and only if

$$\text{span}\left\{ \begin{bmatrix} 0 \\ e_i \\ e_i \end{bmatrix} \middle| a_i = a_{\min} \right\} \cap \operatorname{Ker}(L - m_1) \neq \{0\},$$

where again e_i denotes the i–th canonical basis vector in $\mathcal{K}_{\mathcal{I}}^+$ and $\mathcal{K}_{\mathcal{I}}^-$, respectively, and $m_1 = \|L_+\|$ is the largest positive eigenvalue of L.
Whenever $m_i - \frac{2}{a_{\min}} > 0$, the number κ_i satisfies the lower bound

$$\eta\left(m_i - \tfrac{2}{a_{\min}}, a_{\min}\right) \leq \kappa_i.$$

REMARK 2.5. *For the smallest negative eigenvalue one re–obtains from Theorem 2.4 the lower bound given in [63, Theorem 3.10], which in the above notation is*

$$-\nu(m_1, a_{\min})^2 \leq -\Delta(A, B).$$

The optimality of this bound has been shown in [19, Remark 4.1], by means of the example $L = \mathbb{1}$ and $P = 0$ on a compact graph. An explicit computation of the negative eigenvalues of $-\Delta(L, \mathbb{1})$ exhibits the optimality for this example. Theorem 2.4 gives an easier proof of this optimality. It is sufficient to notice that for any $i \in \mathcal{I}$

$$v_i = \begin{bmatrix} e_i \\ e_i \end{bmatrix} \in \operatorname{Ker}(L - 1),$$

where 1 *is the largest positive eigenvalue of* $L = \mathbb{1}$. *Considering* $-\Delta(\mathbb{1},\mathbb{1})$ *on the interval* $[0,a]$ *one reads from*

$$L(k,\underline{a}) = Q \begin{bmatrix} 1-\kappa\tanh(\kappa a/2) & 0 \\ 0 & 1-\frac{\kappa}{\tanh(\kappa a/2)} \end{bmatrix} Q$$

that if $1-\frac{2}{a} > 0$, *the operator* $-\Delta(\mathbb{1},\mathbb{1})$ *has the two eigenvalues* $-\kappa_1^2 = -\nu(1,a)^2$ *and* $-\kappa_2^2 = -\eta\left(1-\frac{2}{a},a\right)^2$ *with* $-\kappa_1^2 < -\kappa_2^2 < 0$. *Observe that one obtains the bound* $\kappa_1 \leq \nu(1,a)$ *by Theorem 2.4 and* $\kappa_1 \leq \eta(1,a)$ *by Theorem 2.3. A short calculation shows that* $-\eta(1,a)^2 < -\nu(1,a)^2$, *hence Theorem 2.4 provides, in this case, a better lower bound on the bottom of the spectrum than Theorem 2.3.*

An example for the optimality of the lower bound given in Theorem 2.3 is

EXAMPLE 2.6. *Consider on the interval* $[0,a]$ *the operator* $-\Delta(L_c,\mathbb{1})$ *with the non–local boundary conditions defined by*

$$L_c = \frac{c}{2}\cdot\begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix},$$

where one has

$$L_c = Q\begin{bmatrix} 0 & 0 \\ 0 & c \end{bmatrix} Q \quad \text{and hence} \quad L_c(\kappa,a) = Q\begin{bmatrix} -\kappa\tanh(\kappa a/2) & 0 \\ 0 & c-\frac{\kappa}{\tanh(\kappa a/2)} \end{bmatrix} Q.$$

As long as $c-\frac{2}{a} > 0$ *holds, there exists exactly one negative eigenvalue* $\eta(c-\frac{2}{a},a)$ *of* $-\Delta(L_c,\mathbb{1})$, *which is the solution of*

$$\frac{\kappa}{\tanh(\kappa a/2)} = c.$$

The lower bound given in Theorem 2.3 is optimal, whereas the lower bound of Theorem 2.4 predicts a smaller lower bound below zero, even in the case when the operator $-\Delta(L_c,\mathbb{1})$ *is non–negative. Therefore Theorem 2.4 provides less accurate information in this case.*

REMARK 2.7. *The solutions of the transcendent equations given in Theorem 2.3 and Theorem 2.4 are in general only implicitly given. However they can be majorized and minorized by piecewise algebraic functions. Note that*

$$\tanh(y) \geq \begin{cases} \frac{1}{4}y, & 0 \leq y \leq 1, \\ \frac{1}{4}, & y \geq 1, \end{cases}$$

which yields

$$-\kappa\tanh\left(\frac{a}{2}\kappa\right) \leq s(\kappa,a) := -\begin{cases} \frac{1}{4}\frac{a}{2}\kappa^2, & 0 \leq \kappa \leq \frac{2}{a}, \\ \frac{1}{4}\kappa, & \kappa \geq \frac{2}{a}, \end{cases}$$

and hence $m_1 - \tanh(\kappa a_{\min}/2) \leq m_1 + s(\kappa,a_{\min})$ *for* $\kappa \geq 0$. *The unique positive solution of the equation* $m + s(\kappa,a) = 0$ *for* $m > 0$ *is*

$$\xi(m,a) = \begin{cases} \sqrt{\frac{8m}{a}}, & m \leq \frac{1}{2a}, \\ 4m, & m \geq \frac{1}{2a}. \end{cases}$$

Taking advantage of the monotony of the functions involved one concludes that the unique positive solution $\xi(m_1,a_{\min})$ *of* $m_1 + s(\kappa,a_{\min}) = 0$ *is larger than the positive solution* $\nu(m_1,a_{\min})$

of the equation $m_1 - \tanh(\kappa a_{\min}/2) = 0$. *Thus* $-\xi(m_1, a_{\min})^2 \leq -\Delta(A, B)$ *holds and hence also*

$$-\Delta(A,B) \geq -\xi(m_1, a_{\min})^2 \geq \begin{cases} -4\frac{m_1}{a_{\min}}(|\mathcal{E}| + |\mathcal{I}|), & m_1 \leq \frac{1}{2a_{\min}}, \\ -8m_1^2(|\mathcal{E}| + |\mathcal{I}|), & m_1 \geq \frac{1}{2a_{\min}}, \end{cases}$$

holds for $|\mathcal{E}| + |\mathcal{I}| \geq 2$. *This is the lower bound on the spectrum given in [72, Corollary 10]. It has been proven there using quadratic forms associated with self–adjoint Laplace operators and the trace estimate in Lemma 1.13 of Chapter 1. The proof given here exhibits that this lower bound can be re–obtained from the bound given in [63, Theorem 3.10]. More precisely, the bound in [72, Corollary 10] results from a reduction of the bound given in [63, Theorem 3.10].*

The bounds given in Theorem 2.3 and in Theorem 2.4 can be coarsened in order to obtain estimates in terms of affine linear functions. Consider the linear operator

$$R(\kappa, \underline{a}) = L + P^{\perp} M_1(\underline{a}) P^{\perp} - \kappa P^{\perp}, \quad \text{where } M_1(\underline{a}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{\underline{a}} & \frac{1}{\underline{a}} \\ 0 & \frac{1}{\underline{a}} & \frac{1}{\underline{a}} \end{bmatrix},$$

as operator in the Hilbert space $\operatorname{Ran} P^{\perp}$. Since $M(0, \underline{a}) \leq 0$ and $0 \leq M_1(\underline{a})$ in the sense of quadratic forms one has

$$L(0, \underline{a}) \leq L \leq R(0, \underline{a}).$$

Denote by $r_1 \geq \ldots \geq r_n > 0$ the n largest positive eigenvalues of $R(0, \underline{a})$ (counted with multiplicities).

THEOREM 2.8. *Let* $-\Delta(A, B)$ *be self–adjoint. Then the square roots of the absolute values of the negative eigenvalues of* $-\Delta(A, B)$ *obey the two–sided estimates*

$$l_i \leq \kappa_i \leq r_i, \quad \textit{for } 1 \leq i \leq n.$$

Both estimates from below and from above are optimal for star graphs, that is for graphs with $\mathcal{I} = \emptyset$, since then $R(\kappa, \underline{a}) = L(\kappa, \underline{a}) = L - \kappa P^{\perp}$ holds. The estimates given in Theorem 2.8 are compared to the ones given in Theorems 2.3 and 2.4 easy to compute.

When $a_i \to \infty$, uniformly for all $i \in \mathcal{I}$ the lower and upper bounds obtained in Theorem 2.8 converge from below and from above to the positive eigenvalues of L. This follows from

$$\lim_{a_{\min} \to \infty} M(0, \underline{a}) = 0 \quad \text{and} \quad \lim_{a_{\min} \to \infty} M_1(\underline{a}) = 0.$$

Hence, the bounds are improving for large internal edge lengths. In the limit the negative eigenvalues behave like on the disconnected graph on which each internal edge has been replaced by two external edges.

REMARK 2.9. *Since the self–adjoint operators* $-\Delta(A, B)$ *are semi–bounded from below, the operators* $\Delta(A, B)$ *generate strongly continuous quasi-contractive semigroups* $(e^{t\Delta(A,B)})_{t \geq 0}$ *with*

$$\|e^{t\Delta(A,B)}\| \leq e^{\omega t}, \quad t \geq 0,$$

for appropriate ω. *If* $-\Delta(A, B)$ *has negative spectrum then the best possible choice is* $\omega = \kappa_1^2$, *that is the growth bound is exactly the absolute value of the smallest negative eigenvalue, compare for example [33, Corollary IV.3.11]. The above Theorems 2.3, 2.4 and 2.8 provide a priori estimates on this growth bound.*

EXAMPLE 2.10. *Consider the graph that consists of two external edges $\mathcal{E} = \{1,2\}$ connected by an internal edge $I = \{3\}$ of length $\underline{a} = \{a\}$. This means one has two vertices $\partial(1) = \partial_-(3)$ and $\partial(2) = \partial_+(3)$ each of degree two. On each vertex one imposes δ'–interactions with coupling parameter $\gamma \neq 0$, compare for example [2, Chapter I.4] or [72, Section 3.2.3]. These are locally given by the boundary conditions that are defined by*

$$A_\nu = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \quad \textit{and} \quad B_\nu = \begin{bmatrix} 1 & -1 \\ -\gamma & 0 \end{bmatrix}.$$

This gives

$$L = -\frac{1}{\gamma}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \quad \textit{and} \quad P = 0,$$

and

$$M(0,\underline{a}) = \frac{1}{a}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \textit{and} \quad M_1(\underline{a}) = \frac{1}{a}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Consider the operator $-\Delta(L,\mathbb{1})$. The eigenvalues of L are 0 and $-\frac{2}{\gamma}$. The eigenvalues of $L(0,\underline{a}) = L + M(0,\underline{a})$ are

$$0, \quad \frac{-a-\gamma+\sqrt{a^2+\gamma^2}}{a\gamma}, \quad -\frac{a+\gamma+\sqrt{a^2+\gamma^2}}{a\gamma} \quad \textit{and}\ -\frac{2}{\gamma}.$$

Assume for simplicity from now on that $\gamma < 0$. Then there are two positive eigenvalues

$$-\frac{2}{\gamma} \quad \textit{and} \quad -\frac{a+\gamma+\sqrt{a^2+\gamma^2}}{a\gamma}$$

of $L(0,\underline{a})$, and therefore by Proposition 2.1, there are two negative eigenvalues $-\kappa_1^2$ and $-\kappa_2^2$ of $-\Delta(L,\mathbb{1})$. The eigenvalues of $R(0,\underline{a}) = L + M_1(\underline{a})$ are

$$0, \quad \frac{-a+\gamma+\sqrt{a^2+\gamma^2}}{a\gamma}, \quad -\frac{a-\gamma+\sqrt{a^2+\gamma^2}}{a\gamma} \quad \textit{and}\ -\frac{2}{\gamma}.$$

For $\gamma < 0$ there are two positive eigenvalues

$$-\frac{2}{\gamma} \quad \textit{and} \quad -\frac{a-\gamma+\sqrt{a^2+\gamma^2}}{a\gamma}$$

of $R(0,\underline{a})$. Hence by Theorem 2.8

$$-\frac{a+\gamma+\sqrt{a^2+\gamma^2}}{a\gamma} \leq \kappa_2 \leq -\frac{2}{\gamma} \quad \textit{and also} \quad -\frac{2}{\gamma} \leq \kappa_1 \leq -\frac{a-\gamma+\sqrt{a^2+\gamma^2}}{a\gamma}.$$

As already remarked, for $a \to \infty$ the negative eigenvalues resemble the behaviour of the negative eigenvalues of an operator on a disjoint union of star graphs. Here this means that

$$\lim_{a\to\infty} -\kappa_2^2 = -\tfrac{4}{\gamma^2} \quad \textit{and} \lim_{a\to\infty} -\kappa_1^2 = -\tfrac{4}{\gamma^2}.$$

For small edge length the behaviour is more complicated. Since

$$\lim_{a\to 0} -\frac{a+\gamma+\sqrt{a^2+\gamma^2}}{a\gamma} = -\tfrac{1}{\gamma} \quad \textit{and} \quad \lim_{a\to 0} -\frac{a-\gamma+\sqrt{a^2+\gamma^2}}{a\gamma} = \infty$$

one has on the one hand that

$$-\tfrac{4}{\gamma^2} \leq \lim_{a\to 0} -\kappa_2^2 \leq -\tfrac{1}{\gamma^2} \quad \textit{and} \quad -\kappa_1^2 \leq -\tfrac{4}{\gamma^2},$$

but on the other hand it is not clear whether $-\kappa_1^2$ is bounded from below for $a \to 0$. A direct computation gives further information on $-\kappa_1^2$. Consider

$$\mathfrak{l}(\kappa)[x] = \langle L(\kappa,\underline{a})x, x\rangle \quad \textit{with} \quad x = \begin{bmatrix} 0\\1\\1\\0\end{bmatrix},$$

which gives

$$\mathfrak{l}(\kappa)[x] = -\frac{1}{\gamma} - \kappa\tanh(a\kappa/2).$$

The solution of $-\frac{1}{\gamma} - \kappa\tanh(a\kappa/2) = 0$ is $\nu(-\gamma^{-1},a)$, which goes to infinity for $a\to 0$. From the variational characterization of the spectrum of $L(\cdot,\underline{a})$ in the forthcoming Theorem 2.16 it follows that $\nu(-\gamma^{-1},a) \leq \kappa_1$ an therefore

$$\lim_{a\to 0} -\kappa_1^2 = -\infty.$$

REMARK 2.11. *Let be given self–adjoint boundary conditions defined by A, B, a finite graph $\mathcal{G}$ and a family of lengths $\{\underline{a}\}$. One can ask whether the operators $-\Delta(A,B)$ remain uniformly bounded from below when taking the limit $a_{\min}\to 0$. Assume that there is a vector*

$$x \in \textit{span}\left\{ \begin{bmatrix} 0\\ e_i\\ e_i\end{bmatrix} \,\middle|\, a_i = a_{\min}\right\} \cap \operatorname{Ran} P^{\perp} \quad \textit{such that} \quad \langle x, Lx\rangle > 0.$$

Then $\langle x, L(\kappa,\underline{a})x\rangle \leq l_1(\kappa,\underline{a})$ for $\|x\| = 1$, where $l_1(\kappa,\underline{a})$ is the largest positive eigenvalue of $L(\kappa,\underline{a})$. The unique solution of $\langle x, Lx\rangle - \kappa\tanh(a_{\min}\kappa/2) = 0$ is $\nu(\langle x, Lx\rangle, a_{\min})$, which goes to infinity for $a_{\min}\to 0$. From the variational characterization of the singular points of $L(\cdot,\underline{a})$ in the forthcoming Theorem 2.16 it follows that $\nu(\langle x,Lx\rangle, a_{\min}) \leq \kappa_1$ and therefore $\lim_{a\to 0}\kappa_1 = \infty$, and hence the operators are not uniformly bounded from below for $a_{\min}\to 0$. As seen in Example 2.10 this observation applies to δ'–interactions on finite metric graphs with negative coupling parameters γ.

Analogously one obtains if there is a vector

$$x \in \textit{span}\left\{ \begin{bmatrix} 0\\ e_i\\ -e_i\end{bmatrix} \,\middle|\, a_i = a_{\min}\right\} \cap \operatorname{Ran} P^{\perp} \quad \textit{such that} \quad \lim_{a_{\min}\to 0}\langle x, L(0,\underline{a})x\rangle > 0,$$

then the operators $-\Delta(A,B)$ are not uniformly bounded from below for $a_{\min}\to 0$ since $\eta(\langle x, L(0,\underline{a})x\rangle, a_{\min}) \leq \kappa_1$ and $\eta(\langle x, L(0,\underline{a})x\rangle, a_{\min}) \to \infty$ for $a_{\min}\to 0$.

EXAMPLE 2.12. *Consider the same graph as in Example 2.10, but now on each vertex one imposes δ–couplings with coupling parameter $\alpha \neq 0$, compare [2, Chapter I.3] or [72, Section 3.2.1]. These are locally given by the boundary conditions that are defined by*

$$A_\nu = \begin{bmatrix} 1 & -1 \\ -\alpha & 0 \end{bmatrix} \quad \textit{and} \quad B_\nu = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}.$$

This gives

$$P = \frac{1}{2}\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \quad P^\perp = \frac{1}{2}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \quad \textit{and} \quad L = -\frac{\alpha}{2}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}.$$

The matrices $M(0,\underline{a})$ and $M_1(\underline{a})$ are as in Example 2.10, since both depend only on the given metric graph. The operator L considered as an operator in the Hilbert space $\operatorname{Ran} P^\perp$ has the eigenvalue $-\alpha$ of multiplicity two. The operator $L(0,\underline{a}) = L + P^\perp M(0,\underline{a})P^\perp$ has two eigenvalues (each of multiplicity one)

$$-\alpha \quad \textit{and} \quad -\alpha - \frac{1}{a},$$

and the operator $R(0,\underline{a}) = L + P^\perp M_1(\underline{a})P^\perp$ has the two eigenvalues (of multiplicity one)

$$-\alpha \quad \textit{and} \quad -\alpha + \frac{1}{a}.$$

Assume from now on that $\alpha < 0$. For $-\alpha - \frac{1}{a} > 0$ there are by Proposition 2.1 two negative eigenvalues $-\kappa_1^2$ and $-\kappa_2^2$ of $-\Delta(A,B)$ with $A = L + P$ and $B = P^\perp$, and by Theorem 2.8

$$-\alpha - \frac{1}{a} \leq \kappa_2 \leq -\alpha \quad \textit{and}\ -\alpha \leq \kappa_1 \leq -\alpha + \frac{1}{a}.$$

For $-\alpha - \frac{1}{a} \leq 0$ one has only the negative eigenvalue $-\kappa_1^2$ with $-\alpha \leq \kappa_1 \leq -\alpha + \frac{1}{a}$. Now, one can investigate the behaviour of this eigenvalue for $a \to 0$. For this purpose one estimates $L(\kappa,\underline{a}) \leq L + P^\perp Q H(\kappa,\underline{a}) Q P^\perp$, where

$$H(\kappa,\underline{a}) = \begin{bmatrix} -\kappa & 0 & 0 & 0 \\ 0 & -\kappa\tanh(\kappa a/2) & 0 & 0 \\ 0 & 0 & -\kappa\tanh(\kappa a/2) & 0 \\ 0 & 0 & 0 & -\kappa \end{bmatrix}.$$

The eigenvalue (of multiplicity two) of $L + P^\perp Q H(\kappa,\underline{a}) Q P^\perp$ as an operator in $\operatorname{Ran} P^\perp$ is

$$h_\alpha(\kappa, a) = -\alpha - \frac{1}{2}\kappa\tanh(\kappa a/2) - \frac{1}{2}\kappa.$$

The solution of $h_\alpha(\cdot, a) = 0$ converges to -2α for $a \to 0$. Hence κ_1 is bounded for $a \to 0$. In fact, explicit computations show that $\kappa_1 \to -2\alpha$ for $a \to 0$.

2.3. Poincaré type inequalities on compact graphs

Assume now that $(\mathcal{G}, \underline{a})$ is a finite compact metric graph, that is $\mathcal{E} = \emptyset$. Let $-\Delta(A, B)$ be a self–adjoint Laplace operator on this graph. It turns out that the eigenvalue zero of this operator is again related to the function $L(\cdot, \underline{a})$, which appeared in the study of the negative eigenvalues.

PROPOSITION 2.13. *Let $(\mathcal{G}, \underline{a})$ be a compact metric graph and let $-\Delta(A, B)$ be a self–adjoint Laplace operator on the graph. Then zero is an eigenvalue of $-\Delta(A, B)$ if and only if zero is an eigenvalue of the operator $L(0, \underline{a})$ considered as an operator in the Hilbert space $\operatorname{Ran} P^{\perp}$, and for the multiplicty the equality*

$$\dim \operatorname{Ker}\left(-\Delta(A, B)\right) = \dim \operatorname{Ker} L(0, \underline{a})$$

holds. In particular $-\Delta(A, B)$ is strictly positive if and only if $L(0, \underline{a})$ is strictly negative.

EXAMPLE 2.14. *From Remark 2.5 one reads that $-\Delta(\mathbb{1}, \mathbb{1})$ on the interval $[0, a]$ has non–trivial kernel only if $a = 2$. Similarly one obtains for the situation considered in Example 2.6 that $-\Delta(L_c, \mathbb{1})$ has always non–trivial kernel and for $a = \frac{2}{c}$ zero is an eigenvalue of multiplicity two.*

As a consequence of Proposition 2.13 one can prove a criterion for having a Poincaré type estimate on certain subspaces of the Sobolev space $\mathcal{W}$.

THEOREM 2.15. *Let $(\mathcal{G}, \underline{a})$ be a compact metric graph and let P be an orthogonal projector in $\mathcal{K}$, $P^{\perp} = \mathbb{1} - P$. Whenever $\operatorname{Ker} P^{\perp} M(0, \underline{a}) P^{\perp} = \{0\}$ holds, where $P^{\perp} M(0, \underline{a}) P^{\perp}$ is seen as an operator in the Hilbert space $\operatorname{Ran} P^{\perp}$, there exists a constant $C > 0$, where $C = C(P, \underline{a})$, such that*

$$\|\varphi'\|_{\mathcal{H}} \geq C \|\varphi\|_{\mathcal{H}}$$

holds for all

$$\varphi \in \mathcal{W}_P = \{\psi \in \mathcal{W} \mid P\underline{\psi} = 0\}.$$

Consider for example a compact metric graph with at least one vertex of degree one. Impose at all vertices of degree larger than one the so–called Kirchhoff or standard boundary conditions, see for example [63, Example 2.4] and Dirichlet boundary conditions on the vertices of degree one. Then the corresponding Laplacian is strictly positive and consequently a Poincaré type inequality holds.

PROOF OF THEOREM 2.15. The operator $-\Delta(A, B)$ with $A = P$ and $B = P^{\perp}$ is self–adjoint, because $\operatorname{Rank}(P, P^{\perp})$ is maximal and $P\left(P^{\perp}\right)^{*} = PP^{\perp} = 0$. In particular one has $L = 0$. Since $L(0, \underline{a}) = P^{\perp} M(\kappa, \underline{a}) P^{\perp} \leq 0$, it follows from Proposition 2.1 that there are no negative eigenvalues. As $\mathcal{E} = \emptyset$ it follows from the Rellich–Kondrachov Compactness Theorem, see for example [4, Theorem A 5.4], that the embeddings $\mathcal{D} \hookrightarrow \mathcal{W} \hookrightarrow \mathcal{H}$ are compact. Hence the spectrum of $-\Delta(A, B)$ is purely discrete and under the assumption $\operatorname{Ker} L(0, \underline{a}) = \{0\}$, where $L(0, \underline{a})$ is seen as an operator in $\operatorname{Ran} P^{\perp}$, the operator $-\Delta(A, B)$ is strictly positive by Proposition 2.13, and the infimum of the numerical range is attained by the lowest eigenvalue $\lambda_1 = \min \sigma(-\Delta(A, B)) > 0$. Consequently one has

$$\langle -\Delta(A, B)\varphi, \varphi \rangle \geq \lambda_1 \langle \varphi, \varphi \rangle, \quad \text{for all} \quad \varphi \in \operatorname{Dom}(-\Delta(A, B)).$$

The operator $-\Delta(A, B)$ is uniquely defined by the sesquilinear form $\bar{\delta}_P$ which is given by $\bar{\delta}_P[\varphi, \psi] = \langle \varphi', \psi' \rangle$ on the form domain $\operatorname{dom} \bar{\delta}_P = \{\psi \in \mathcal{W} \mid P\underline{\psi} = 0\}$, see [72, Theorem 9].

Since the operator domain of $-\Delta(A,B)$ is a core of $\operatorname{dom}\bar{\delta}_P$ by the first representation theorem, see for example [58, Chapter VI §2, Theorem 2.1], the inequality

$$\|\varphi'\|^2 = \langle\varphi',\varphi'\rangle \geq \lambda_1\langle\varphi,\varphi\rangle$$

holds even for all $\varphi \in \operatorname{dom}\delta_P = \mathcal{W}_P$, compare [58, Chapter VI §2, Corollary 2.3]. The positive square root k_1 of the smallest positive eigenvalue $\lambda_1 = k_1^2$ of $-\Delta(A,B)$ is a solution of $\det\left(PX(k,\underline{a}) + ikP^{\perp}Y(k,\underline{a})\right) = 0$, see for example [63, Lemma 3.1], and therefore it depends only on P and $\underline{a}$. □

PROOF OF PROPOSITION 2.13. Eigenfunctions to the eigenvalue zero are piecewise affine. This gives the *Ansatz*

$$\psi_0(x_j) = \alpha_j^0 + \beta_j^0 x_j, \quad j\in\mathcal{I}$$

with traces

$$\underline{\psi_0(\cdot)} = X_0\left(\underline{a}\right)\begin{bmatrix}\{\alpha_j^0(i\kappa)\}_{j\in\mathcal{I}}\\ \{\beta_j^0(i\kappa)\}_{j\in\mathcal{I}}\end{bmatrix}, \qquad \underline{\psi_0(\cdot)'} = Y_0\left(\underline{a}\right)\begin{bmatrix}\{\alpha_j^0(i\kappa)\}_{j\in\mathcal{I}}\\ \{\beta_j^0(i\kappa)\}_{j\in\mathcal{I}}\end{bmatrix},$$

where

$$X_0\left(\underline{a}\right) = \begin{bmatrix}\mathbb{1} & 0\\ \mathbb{1} & \underline{a}\end{bmatrix} \quad\text{and}\quad Y_0\left(\underline{a}\right) = \begin{bmatrix}0 & \mathbb{1}\\ 0 & -\mathbb{1}\end{bmatrix}.$$

Consequently zero is an eigenvalue of the self–adjoint operator $-\Delta(A,B)$ if and only if

$$\det\left(AX_0(\underline{a}) + BY_0(\underline{a})\right) = 0.$$

As $X_0\left(\underline{a}\right)$ is invertible this condition is equivalent to

$$\det(A + BM_0(\underline{a})) = 0, \quad\text{where}\quad M_0(\underline{a}) = Y_0(\underline{a})X_0(\underline{a})^{-1}.$$

Note that $M_0(\underline{a}) = M(0,\underline{a})$, where $M(0,\underline{a})$ is the operator from equation (28). Hence $-\Delta(A,B)$ has eigenvalue zero if and only if zero is an eigenvalue of $L(0,\underline{a})$ and the multiplicities of both agree.

Since the spectrum of $-\Delta(A,B)$ is purely discrete, the operator $-\Delta(A,B)$ is strictly positive if and only if zero is no eigenvalue and there are no negative eigenvalues. By Proposition 2.1 and the above calculation this is the case if and only if $L(0,\underline{a})$ considered as an operator in the Hilbert space $\operatorname{Ran}P^{\perp}$ is strictly negative. □

2.4. Variational methods and proofs

An appropriate method to deal with the negative eigenvalues of $-\Delta(A,B)$ is the variational principle developed by P. A. Binding, D. Eschwé and H. Langer in [16], which has been extended by D. Eschwé and M. Langer in [34]. It has been successfully applied in the article [12] to compute the number of negative eigenvalues. Some facts are going to be respeated here as far as necessary.

Let $I := [\alpha,\beta) \subset \mathbb{R}$ be a real (not necessarily bounded) interval and and X a finite dimensional Hilbert space. Denote by $\operatorname{Herm}(X)$ the set of all Hermitian operators in X. The spectrum of a function

$$T(\cdot)\colon I \to \operatorname{Herm}(X), \quad \lambda \mapsto T(\lambda)$$

is defined by

$$\sigma(T(\cdot)) := \{\lambda\in\mathbb{C} \mid \det T(\lambda) = 0\}.$$

The variational principle for operator valued functions is inspired by the $\min - \max$ principle for the linear eigenvalue problem. It has been exhibited in [16] that spectral points of more general operator valued functions can be found similarly to eigenvalues of linear self–adjoint operators as long as some key–properties are assumed. The results obtained in [34] are reduced and reformulated for the purpose of this work.

THEOREM 2.16 (compare [34, Theorem 2.1]). *Let* $T\colon [\alpha, \beta) \to \mathrm{Herm}\,(X)\,, \lambda \mapsto T(\lambda)$ *be*

(1) norm–continuous and

(2) assume that for each $x \in X \setminus \{0\}$*, the function*

$$\mathfrak{t}[x](\lambda) := \langle T(\lambda)x, x\rangle$$

is decreasing at value zero, which means that from $\mathfrak{t}[x](\lambda_0) = 0$ *it follows that for* $\lambda < \lambda_0$*,* $\mathfrak{t}[x](\lambda) > 0$ *and for* $\lambda > \lambda_0$*,* $\mathfrak{t}[x](\lambda) < 0$ *holds.*

Denote by N_- *the number of negative eigenvalues of* $T(\alpha)$*, by* N_+ *the number of positive eigenvalues of* $T(\alpha)$ *and by* N_0 *the dimension of* $\mathrm{Ker}\,T(\alpha)$*. Assume furthermore that*

(3) *there is a* $\gamma \in [\alpha, \beta)$ *such that* $T(\gamma) < 0$*.*

Then $\sigma(T(\cdot))$ *consists of* N_+ *eigenvalues* $\lambda_1 \leq \ldots \leq \lambda_n \leq \ldots \leq \lambda_{N_+}$ *(counted with multiplicities) with* $\lambda_n > \alpha$*, and* α *is an eigenvalue with multiplicity* N_0*. The eigenvalues* λ_n *are given by*

$$\lambda_n = \min_{\dim S = N_- + N_0 + n} \max_{x \in S} \rho(x) \quad \textit{and} \quad \lambda_n = \max_{\dim S = n + N_- + N_0 + 1} \min_{x \perp S} \rho(x),$$

where the generalized Rayleigh functional $\rho(x)$ *is the unique solution of*

$$\mathfrak{t}[x](\cdot) = 0, \quad \textit{for } \|x\| = 1$$

and if there is no solution one sets $\rho(x) = -\infty$*.*

The proof of the above theorem is based on the study of the function

$$\phi\colon [\alpha, \beta) \to \mathbb{N},\ \lambda \mapsto \phi(\lambda) := \dim T_-(\lambda),$$

where $T_-(\lambda)$ denotes the strictly negative part of $T(\lambda)$. This function is monotone increasing and left continuous and the height of jumps of κ gives the multiplicity of an eigenvalue of $T(\cdot)$. An important corollary for the construction of appropriate comparison operators is the following theorem. It allows one to compare two operator valued functions to each other whenever an inequality in terms of quadratic forms holds.

THEOREM 2.17 (compare [34, Corollary 2.12]). *Let* $T(\cdot)$ *and* $S(\cdot)$ *be two operator valued functions defined on* $[\alpha, \beta)$ *that satisfy the assumptions of Theorem 2.16. Denote by* $\lambda_1^T \leq \ldots \leq \lambda_{N_+}^T$ *and* $\lambda_1^S \leq \ldots \leq \lambda_{M_+}^S$ *the eigenvalues (counted with multiplicities) of* $T(\cdot)$ *and* $S(\cdot)$ *in* (α, β)*, respectively. Assume that*

$$\mathfrak{t}[x](\lambda) \leq \mathfrak{s}[x](\lambda)$$

holds for all $x \in X$ *and all* $\lambda \in [\alpha, \beta)$*. Then one has* $N_+ \leq M_+$ *and for the* N_+ *largest eigenvalues of* $S(\cdot)$ *and* $T(\cdot)$ *(counted with multiplicities) it follows that*

$$\lambda_n^T \leq \lambda_n^S.$$

LEMMA 2.18. *The operator valued function*

$$L(\cdot,\underline{a})\colon [0,\infty) \to \operatorname{Herm}(\operatorname{Ran} P^{\perp}), \quad \kappa \mapsto L(\kappa,\underline{a}),$$

satisfies the assumptions of Theorem 2.16.

Multiplying $L(\kappa,\underline{a})$ from both sides with the symmetry Q one obtains the unitarily equivalent operator

$$L_Q(\kappa,\underline{a}) = QLQ + QP^{\perp}QD(\kappa,\underline{a})QP^{\perp}Q,$$

which is considered as an operator in the space $\operatorname{Ran} QP^{\perp}Q$. The operator $P_Q := QPQ$ is an orthogonal projector with orthogonal complement $P_Q^{\perp} := \mathbb{1} - P_Q$, $P_Q^{\perp} = QP^{\perp}Q$ and $L_Q := QLQ$ defines an operator in the space $\operatorname{Ran} P_Q^{\perp}$, which is isometrically isomorphic to $\operatorname{Ran} P^{\perp}$.

PROOF. The function $L(\cdot,\underline{a})$ is norm–continuous, because the function $D(\cdot,\underline{a})$ is already norm–continuous. It remains to prove that the function $\mathfrak{l}[x](\cdot) = \langle L(\cdot,\underline{a})x,x\rangle$ is decreasing at the point zero for all $x \in \operatorname{Ran} P^{\perp}$. This is implied by the statement that the function $\mathfrak{l}_Q[x](\cdot) = \langle L_Q(\cdot,\underline{a})x,x\rangle$ is strictly decreasing for all $x \in \operatorname{Ran} P_Q^{\perp}$ with $\|x\| = 1$. Since $D(\cdot,\underline{a})$ is a diagonal matrix with strictly decreasing functions on the diagonal, the function defined by $\langle (P_Q + L_Q + D(\cdot,\underline{a}))x,x\rangle$ is strictly decreasing for any $x \in \mathcal{K}$, in particular for all $x \in \operatorname{Ran} P_Q^{\perp}$. Furthermore, for any $x \in \operatorname{Ran} P_Q^{\perp} \setminus \{0\}$ one has $\langle L(\kappa,\underline{a})x,x\rangle \to -\infty$ for $\kappa \to \infty$, since already $\langle D(\kappa,\underline{a})x,x\rangle \to -\infty$ for $\kappa \to \infty$, and thus, also Assumption (3) of Theorem 2.16 is fulfilled. $\square$

One considers different operator valued functions in order to compare them to $L(\cdot,\underline{a})$ – or equivalently to $L_Q(\cdot,\underline{a})$ – by means of Theorem 2.17. For this purpose take into account

LEMMA 2.19. *Let* $0 < a_{\min} \leq a_i \leq a_{\max}$*, then the following elementary estimates hold for* $\kappa \geq 0$*,*

$$-\kappa\tanh\left(\tfrac{\kappa a_{\max}}{2}\right) \leq -\kappa\tanh\left(\tfrac{\kappa a_i}{2}\right) \leq -\kappa\tanh\left(\tfrac{\kappa a_{\min}}{2}\right), \tag{29}$$

$$-\frac{\kappa}{\tanh\left(\frac{\kappa a_{\min}}{2}\right)} \leq -\frac{\kappa}{\tanh\left(\frac{\kappa a_i}{2}\right)} \leq -\frac{\kappa}{\tanh\left(\frac{\kappa a_{\max}}{2}\right)}, \tag{30}$$

$$-\frac{\kappa}{\tanh\left(\frac{\kappa a_{\max}}{2}\right)} + \frac{2}{a_{\max}} \leq -\frac{\kappa}{\tanh\left(\frac{\kappa a_i}{2}\right)} + \frac{2}{a_i} \leq -\frac{\kappa}{\tanh\left(\frac{\kappa a_{\min}}{2}\right)} + \frac{2}{a_{\min}}, \tag{31}$$

$$-\frac{\kappa}{\tanh\left(\frac{\kappa a_i}{2}\right)} < -\kappa \leq -\kappa\tanh\left(\tfrac{\kappa a_i}{2}\right), \tag{32}$$

$$-\kappa \leq -\kappa\tanh\left(\tfrac{\kappa a_i}{2}\right) \leq -\frac{\kappa}{\tanh\left(\frac{\kappa a_i}{2}\right)} + \frac{2}{a_i}. \tag{33}$$

In (32) *and* (33) *equality holds only if* $\kappa = 0$*. In* (29) *equality holds only if* $\kappa = 0$ *or if* $a_i = a_{\min} = a_{\max}$*. In* (30) *and* (31) *equality holds only if* $a_i = a_{\min} = a_{\max}$*.*

PROOF. The function $-\tanh(y)$ is strictly decreasing for $y \geq 0$. Therefore plugging in

$$y_1 := \frac{\kappa a_{\min}}{2} \leq \frac{\kappa a_i}{2} =: y_2 \tag{34}$$

and multiplying by $\kappa \geq 0$ yields inequality (29). With a similar calculation one obtains (30). Note that for fixed $\kappa > 0$ the function

$$a \mapsto \frac{-\kappa}{\tanh\left(\frac{\kappa a}{2}\right)} + \frac{2}{a}, \quad a > 0,$$

is strictly decreasing, and therefore inequality (31) holds. Inequality (32) follows already from the inequality $\tanh(y) < 1$ for $y \geq 0$. The last inequality (33), substituting $y = \frac{a_i \kappa}{2}$, is equivalent to $-y\tanh^2(y) \leq -y + \tanh(y)$ for $y \geq 0$. This in turn is true, because

$$\begin{aligned}
&\frac{d}{dy}\left(-y\tanh^2(y)\right) = -\tanh^2(y) - 2y\tanh(y)(1-\tanh(y)^2),\\
&\frac{d}{dy}\left(-y+\tanh(y)\right) = -\tanh^2(y)
\end{aligned}$$

and hence

$$\frac{d}{dy}\left(-y\tanh^2(y)\right) \leq \frac{d}{dy}\left(-y+\tanh(y)\right), \quad \text{for } y \geq 0,$$

and, in addition, for the initial values at $y = 0$ the equality $-0\tanh^2(0) = 0 = -0 + \tanh(0)$ holds. ☐

PROOF OF THEOREM 2.3. Taking into account

$$\begin{aligned}
L_Q(\kappa, \underline{a}) =& L_Q + P_Q^\perp D(\kappa, \underline{a}) P_Q^\perp\\
=& L_Q + P_Q^\perp D(0, \underline{a}) P_Q^\perp + P_Q^\perp\left(D(\kappa, \underline{a}) - D(0, \underline{a})\right) P_Q^\perp\\
=& L_Q(0, \underline{a}) + P_Q^\perp\left(D(\kappa, \underline{a}) - D(0, \underline{a})\right) P_Q^\perp
\end{aligned}$$

one considers the operator valued functions

$$L_1(\kappa, \underline{a}) = L_Q(0, \underline{a}) - \left(\frac{\kappa}{\tanh(\kappa a_{\min}/2)} - \frac{2}{a_{\min}}\right) P_Q^\perp$$

and

$$L_2(\kappa, \underline{a}) = L_Q(0, \underline{a}) - \kappa P_Q^\perp.$$

By (31) and (33) one has

$$-\kappa\mathbb{1} \leq D(k, \underline{a}) - D(0, \underline{a}) \leq -\left(\frac{\kappa}{\tanh(\kappa a_{\min}/2)} - \frac{2}{a_{\min}}\right)\mathbb{1} \quad \text{for } \kappa \geq 0,$$

and hence

$$L_2(\kappa, \underline{a}) \leq L_Q(\kappa, \underline{a}) \leq L_1(\kappa, \underline{a}) \quad \text{for } \kappa \geq 0. \tag{35}$$

The operator valued functions $L_1(\cdot, \underline{a})$ and $L_2(\cdot, \underline{a})$ are strictly decreasing and continuous. The proof of this is analogue to the one of Lemma 2.18. Furthermore one has for any $x \in \operatorname{Ran} P^\perp$ with $\|x\| = 1$ that $\langle x, L_j(\kappa, \underline{a})x\rangle \to -\infty$ for $\kappa \to \infty$ with $j = 1, 2$. Hence $L_1(\cdot, \underline{a})$ and $L_2(\cdot, \underline{a})$ satisfy the assumptions of Theorem 2.17.

By construction, for $\kappa > 0$ the operator valued function $L_2(\cdot, \underline{a})$ has n eigenvalues, which are the n positive eigenvalues l_i of $L_2(0, \underline{a}) = L_Q(0, \underline{a})$, $i = 1, \ldots, n$. Recall that by Proposition 2.1 the number of negative eigenvalues of $-\Delta(A, B)$ counted with multiplicities is equal to n. By definition, for $\kappa > 0$ the function $L_1(\cdot, \underline{a})$ has n eigenvalues, because $L_1(0, \underline{a}) =$

$L_Q(0,\underline{a})$, and these are exactly $\eta(l_i, a_{\min})$, $i=1,\dots,n$. Theorem 2.17 delivers the estimates for the numbers κ_i.

To prove the optimality of the resulting lower bound on the spectrum one considers the spaces

$$E_{a_{\min}} := \operatorname{span}\left\{ \begin{bmatrix} 0 \\ 0 \\ e_i \end{bmatrix} \middle| a_i = a_{\min} \right\} \quad \text{and} \quad \operatorname{Ker}(L_Q(0,\underline{a}) - l_1),$$

which is the eigenspace of $L_Q(0,\underline{a})$ to its largest positive eigenvalue l_1. One proves that the bound $\eta(l_i, a_{\min})$ is optimal if and only if there is a vector $x \neq 0$ with

$$x \in \operatorname{Ker}(QLQ - l_1) \cap E_{a_{\min}}.$$

Assume that $x \in \operatorname{Ker}(L_Q(0,\underline{a}) - l_1) \cap E_{a_{\min}}$ with $\|x\| = 1$, then

$$\mathfrak{l}_Q[x](\kappa) = \langle x, L_Q(\kappa,\underline{a})x\rangle = l_1 + \frac{2}{a_{\min}} - \frac{\kappa}{\tanh(\kappa a_{\min}/2)}.$$

Denote the unique zero of this function by κ_0, and observe that $\kappa_0 = \eta(l_1, a_{\min})$. Assume that $y \neq 0$ and denote furthermore by $\rho(y)$ the solution of $\mathfrak{l}_Q[y](\cdot) = 0$ or, if there is no solution of this, one sets $\rho(y) = -\infty$. Note that for all $y \in \operatorname{Ran} P_Q^{\perp}$ with $\|y\| = 1$ one has using (29), (31) and (32)

$$\begin{aligned} \mathfrak{l}_Q[y](\kappa_0) =& \langle y, L_Q(0,\underline{a})y\rangle + \langle P_Q^{\perp} y, (D(\kappa_0,\underline{a}) - D(0,\underline{a}))\, P_Q^{\perp} y\rangle \\ \leq & l_1 + \frac{2}{a_{\min}} - \frac{\kappa_0}{\tanh(\kappa_0 a_{\min}/2)} = \mathfrak{l}_Q[x](\kappa_0) = 0 \end{aligned}$$

and hence $\rho(y) \leq \rho(x)$. Therefore

$$\kappa_0 = \rho(x) = \max_{\substack{y \in \operatorname{Ran} P_Q^{\perp} \\ \|y\|=1}} \rho(y),$$

and by the variational characterisation of the eigenvalues given in Theorem 2.16 it follows that κ_0 is indeed a zero of $\det L_Q(\cdot,\underline{a})$ and hence $-\kappa_0^2$ is the lowest eigenvalue of $-\Delta(A,B)$.

Conversely, assume that the bound $\eta(l_1, a_{\min})$ is taken, which means that there exists a vector $x \in \operatorname{Ran} P^{\perp}$ with $\|x\| = 1$ such that $L_Q(\eta(l_1, a_{\min}),\underline{a})x = 0$. Consider again the function

$$\mathfrak{l}_Q[x](\cdot) = \langle L_Q(\cdot,\underline{a})x, x\rangle.$$

First, one shows

$$\mathfrak{l}_Q[x](0) = l_1.$$

Assume that $\mathfrak{l}_Q[x](0) < l_1$. Since $D(\kappa,\underline{a}) - D(0,\underline{a}) \leq \frac{2}{a_{\min}} - \frac{\kappa}{\tanh(\kappa a_{\min}/2)}$ for $\kappa \geq 0$ it would follow that the unique solution of $\mathfrak{l}_Q[x](\kappa) = 0$ is smaller than $\eta(l_1, a_{\min})$, which contradicts the assumption.

Assume conversely that $\mathfrak{l}_Q[x](0) > l_1$. This is a contradiction to the inequality $L_Q(\kappa,\underline{a}) \leq L_1(\kappa)$ for $\kappa \geq 0$ and the claim follows.

By what was just proven and the classical $\min-\max$-principle

$$\mathfrak{l}_Q[x](0) = l_1 = \max_{\substack{y \in \operatorname{Ran} P_Q^{\perp} \\ \|y\|=1}} \langle y, L(0,\underline{a})y\rangle$$

and the maximum is attained for $y = x$, hence $x \in \operatorname{Ker}(L_Q(0, \underline{a}) - l_1)$.

Assume now that $x \notin E_{a_{\min}}$. By (31) and (33) one has

$$\langle (D(\kappa, \underline{a}) - D(0, \underline{a}))x, x\rangle \leq \frac{2}{a_{\min}} - \frac{\kappa}{\tanh(\kappa a_{\min}/2)}, \quad \text{for } \kappa > 0 \text{ and } \|x\| = 1,$$

and that equality holds only if $x \in E_{a_{\min}}$. Hence $\mathfrak{l}_Q[x](\kappa) < l_1 - \frac{2}{a_{\min}} - \frac{\kappa}{\tanh(\kappa a_{\min}/2)}$ would hold for $\kappa > 0$ and it would follow that the unique solution of $\mathfrak{l}_Q[x](\kappa) = 0$ was smaller than $\eta(l_1, a_{\min})$. This is a contradiction and hence $x \in E_{a_{\min}}$. Note that

$$QE_{a_{\min}} := \operatorname{span}\left\{ \begin{bmatrix} 0 \\ e_i \\ -e_i \end{bmatrix} \middle| a_i = a_{\min} \right\}.$$

□

PROOF OF THEOREM 2.4. Define the comparison operator

$$L_3(\kappa, a_{\min}) = L_Q - \kappa \tanh(\kappa a_{\min}/2) P_Q^{\perp}.$$

By definition the first n positive eigenvalues of $L_3(\cdot, \underline{a})$ are $\nu(m_i, a_{\min})$, for $i = 1, \ldots, n$. It is straightforward to verify that the operator valued function $L_3(\cdot, \underline{a})$ satisfies the assumptions of Theorem 2.16. From the inequalities (29) and (32) one reads

$$D(k, \underline{a}) \leq -\kappa \tanh(\kappa a_{\min}/2)\mathbb{1} \quad \text{for } \kappa \geq 0,$$

and consequently

$$L_Q(\kappa, \underline{a}) \leq L_3(\kappa, \underline{a}), \quad \text{for } \kappa \geq 0.$$

Applying Theorem 2.17 proves the first part of the theorem.

To prove the optimality of the resulting lower bound on the spectrum one considers the spaces

$$F_{a_{\min}} := \operatorname{span}\left\{ \begin{bmatrix} 0 \\ e_i \\ 0 \end{bmatrix} \middle| a_i = a_{\min} \right\} \quad \text{and} \quad \operatorname{Ker}(L_Q - m_1),$$

which is the eigenspace of L_Q to its largest positive eigenvalue m_1. One proves as in the proof of Theorem 2.3 that the bound $-\nu(m_i, a_{\min})^2$ is optimal if and only if there is a vector $x \neq 0$ with

$$x \in \operatorname{Ker}(L_Q - m_1) \cap F_{a_{\min}}.$$

To prove the lower bounds on the numbers κ_i. consider the function $L_4(\cdot, \underline{a})$ defined by

$$L_4(\kappa, \underline{a}) = L_Q - \left(\frac{\kappa}{\tanh(\kappa a_{\min}/2)} \right) P_Q^{\perp}, \quad \kappa \geq 0.$$

For each m_i with $m_i > \frac{2}{a_{\min}}$ there is an eigenvalue of $L_4(\cdot, \underline{a})$, which is by definition $\eta(m_i - \frac{2}{a_{\min}}, a_{\min})$. Since by (30) and (32)

$$\frac{-\kappa}{\tanh(\kappa a_{\min}/2)}\mathbb{1} \leq D(k, \underline{a}) \quad \text{for } \kappa \geq 0,$$

also

$$L_4(\kappa, \underline{a}) \leq L_Q(\kappa, \underline{a}), \quad \text{holds for } \kappa \geq 0,$$

and the claim follows with Theorem 2.17. □

PROOF OF THEOREM 2.8. The proof of Theorem 2.8 takes advantage of the estimates

$$-\kappa + \frac{2}{a} \geq -\kappa \tanh\left(\frac{a}{2}\kappa\right) \quad \text{for } \kappa \geq 0.$$

Substituting $y = \frac{a\kappa}{2}$, this is equivalent to $y - 1 \leq y\tanh(y)$ for $y \geq 0$. Together with (32) this yields for $\kappa \geq 0$ the inequality

$$D(\kappa, \underline{a}) \leq R_1(\kappa, \underline{a}), \quad \text{where } R_1(\kappa, \underline{a}) = \begin{bmatrix} -\kappa & 0 & 0 \\ 0 & -\kappa + \frac{2}{\underline{a}} & 0 \\ 0 & 0 & -\kappa \end{bmatrix}.$$

This in turn gives for $\kappa \geq 0$ together with the lower estimates from Theorem 2.3 the inequality

$$L_2(\kappa, \underline{a}) \leq L_Q(\kappa, \underline{a}) \leq QLQ + P_Q^{\perp} R_1(\kappa, \underline{a}) P_Q^{\perp}.$$

Note that the positive eigenvalues of the operator valued function

$$L_5(\cdot, \underline{a})\colon [0, \infty) \to \operatorname{Herm}(\operatorname{Ran} P_Q^{\perp}), \quad \kappa \mapsto QLQ + P_Q^{\perp} R_1(\kappa, \underline{a}) P_Q^{\perp}$$

agree with the positive eigenvalues of $R(0, \underline{a})$. Applying Theorem 2.17 yields the claim. □

CHAPTER 3

Mixed dynamics: diffusion and transport

The most studied problems on finite metric graphs concern homogeneous dynamical processes. This means on each edge the dynamics is modelled for example as a transport, as a diffusion or as a wave evolution. However, many physical models consist of coexisting, interacting processes of different types. On different edges a different kind of dynamics may take place; or else, one may introduce auxiliary edges in the model in order to describe certain phenomena, like time–delays, in a more efficient way.

The aim of this chapter is to discuss a system on a metric graph which satisfies the one–dimensional heat equation on some edges and the one–dimensional transport equation on the rest of the edges. The Cauchy problem for this mixed problem can be expressed as

$$\tag{36} \begin{cases} \left(\dfrac{\partial}{\partial t} - A\right) u(x,t) = 0, \\ \\ u(\cdot,0) = u_0, \end{cases} \qquad \text{for } t \geq 0 \quad \text{with} \quad A = \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & -\frac{d}{dx} \end{bmatrix}.$$

For simplicity assume that the underlying graph is compact.

It is assumed that the interactions of the different subsystems are taking place only at the vertices, and therefore the coupling is implemented by imposing boundary conditions at the vertices of the graph. In this way the system can be translated into an abstract Cauchy problem involving an operator defined by the differential expression A along with appropriate boundary conditions. The class of boundary conditions introduced here delivers quasi–m–dissipative operators and hence infinitesimal generators of quasi–contractive semigroups. This gives rise to solutions to the initial value problem (36) in terms of semigroups.

On metric graphs the diffusion and the transport equation are usually considered independently and as different topics. Some pioneering investigations on systems of transport equations on metric graphs have been commenced by M. Kramar and E. Sikolya in the article [69]. Questions related to the diffusion equation on metric graphs have been discussed also in Chapter 1, and further references on this topic are given there. The goal is to connect these two theories. The easiest case of the coupling of *one* diffusion and *one* transport equation have been studied already by F. Gastaldi and A. Quarteroni in the article [39], where certain vector valued functions have been considered.

One motivation for introducing this setting arises from some biomathematical considerations. It is known that electric signal coming from a neuron undergoes a certain synaptic delay before reaching another neuron, and it cannot turn back. This suggests to model this process by a system of diffusion equations – in the dendrites or axons – and transport equations – in the synapse. In specific situations it turns out that the setting considered here can be adapted to discuss coupled systems of diffusion equations with boundary delays. While the proposed dynamics actually seem to reflect the observed phenomena, it is very difficult to make an educated guess when it comes to propose *natural* transmission conditions. It seems that the search for, in some sense *natural*, transmission conditions is much less trivial in the mixed case than in the case of purely diffusive or pure transport–like systems. This unexpected difficulty is discussed in some detail in [39, § 2].

This chapter is based on a joint work with Delio Mugnolo and the content is mainly taken from our common work which is already published in the article [54]. The chapter is organized as follows: in the subsequent section boundary conditions are introduced that define quasi–m–dissipative realizations of the differential operator A. This is the main result of this chapter, because this implies that the time–dependent problem given in (36) together with appropriate boundary conditions is well posed. Thereafter, the spectral theory of these operators is developed, followed by the discussion of a simplified model of a dendro–dendritical chemical synapse, which fits into the presented framework. Finally, other examples of mixed dynamics on metric graphs are discussed briefly.

3.1. Maximal dissipative boundary conditions

Consider a finite compact graph $\mathcal{G} = (V, \mathcal{I}, \partial)$, and for the purposes of this chapter a partition of the set of edges

$$\mathcal{I} = \mathcal{I}_d \dot{\cup} \mathcal{I}_t \tag{37}$$

into two disjoint subsets $\mathcal{I}_d$ and $\mathcal{I}_t$ representing the edges on which *diffusion* and *transport* phenomena are going to take place, respectively. Denote by $\mathcal{I}_d = \{\mathsf{e}_{d1}, \dots, \mathsf{e}_{dD}\}$ the *diffusion edges* and by $\mathcal{I}_t = \{\mathsf{e}_{t1}, \dots, \mathsf{e}_{tT}\}$ the *transport edges* of the metric graph. To each edge e_{di} or e_{tj} a length a_{di} or a_{tj}, respectively, is associated with. This delivers the length vector $\underline{a}$. Consider the metric graph $(\mathcal{G}, \underline{a})$.

The partition (37) gives rise to the definition of the two subgraphs

$$\mathcal{G}_d = (V_d, \mathcal{I}_d, \partial_d) \quad \text{and} \quad \mathcal{G}_t = (V_t, \mathcal{I}_t, \partial_t),$$

where ∂_d and ∂_t are the restrictions of ∂ to $\mathcal{I}_d$ and $\mathcal{I}_t$, respectively. Accordingly V_d, and V_t are the ranges of ∂_d and ∂_t, respectively. Each of the subgraphs $\mathcal{G}_d$ and $\mathcal{G}_t$ is endowed with the metric structure,

$$\underline{a}_d = \{a_{di}\}_{i=1,\dots,D} \quad \text{and} \quad \underline{a}_t = \{a_{tj}\}_{j=1,\dots,T}.$$

One considers the Hilbert space $\mathcal{H} \equiv \mathcal{H}(\mathcal{I}, \underline{a})$ of square integrable functions defined on the intervals associated with the edges. The subdivision (37) induces the partition

$$\mathcal{H} = \mathcal{H}_d \oplus \mathcal{H}_t, \tag{38}$$

where $\mathcal{H}_d = \mathcal{H}(\mathcal{I}_d, \underline{a}_d)$ and $\mathcal{H}_t = \mathcal{H}(\mathcal{I}_t, \underline{a}_t)$ are the Hilbert spaces of square integrable functions on the subgraphs $(\mathcal{G}_d, \underline{a}_d)$ and $(\mathcal{G}_t, \underline{a}_t)$. Clearly any element $u \in \mathcal{H}$ can be written with respect to this decomposition as

$$u = \begin{bmatrix} u_d \\ u_t \end{bmatrix}, \quad \text{where } u_d \in \mathcal{H}_d \text{ and } u_t \in \mathcal{H}_t.$$

Consider the space $\mathcal{W}$ defined in (5), which also has a subdivision according to the subdivision of $\mathcal{H}$,

$$\mathcal{W} = \mathcal{W}_d \oplus \mathcal{W}_t, \quad \text{where} \quad \mathcal{W}_d = \mathcal{W}(\mathcal{I}_d) \text{ and } \mathcal{W}_t = \mathcal{W}(\mathcal{I}_t).$$

The space $\mathcal{D}_d = \mathcal{D}(\mathcal{I}_d)$ defined in (6) is considered only for the diffusion edges.

3.1.1. Boundary conditions. Now, in the Hilbert space $\mathcal{H} = \mathcal{H}_d \oplus \mathcal{H}_t$ one considers the diagonal block operator matrix A which is given with respect to the decomposition (38) by

$$A = \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & -\frac{d}{dx} \end{bmatrix}, \quad \text{that is} \quad Au = A \begin{bmatrix} u_d \\ u_t \end{bmatrix} = \begin{bmatrix} u_d'' \\ -u_t' \end{bmatrix}. \tag{39}$$

The operator A is defined on the (maximal) domain

$$\mathrm{Dom}(A) = \mathcal{D}_d \oplus \mathcal{W}_t.$$

Denote by A^0 the restriction of A to the (minimal) domain

$$\mathrm{Dom}(A^0) = \mathcal{D}_d^0 \oplus \mathcal{W}_t^0.$$

Recall that an operator T is called (quasi–)m–dissipativity if and only if $-T$ is (quasi–)m–accretive. The notion of (quasi–)m–accretivity has been discussed in Chapter 1 already. Here, certain m–dissipative realizations $\widetilde{A}$ of A with

$$A^0 \subset \widetilde{A} \subset A$$

are introduced. That A^0 and A are the extreme relevant cases follows from the observation that both decouple the edges. Note that the operator A^0 is the direct sum of a symmetric and a skew–symmetric operator. Therefore it might serve also as a model problem for more general situations.

REMARK 3.1. *It has been observed in Chapter 1 that all quasi–m–dissipative realizations of the second derivative operator acting on the space of square integrable functions over a metric graph with m edges, each identified with an interval $(0, 1)$, can be parametrized by a family of boundary conditions*

$$P^\perp \begin{bmatrix} -u'(0) \\ u'(1) \end{bmatrix} + (L + P) \begin{bmatrix} u(0) \\ u(1) \end{bmatrix} = 0,$$

where P is any orthogonal projection of $\mathbb{C}^{2m}$ and L is any matrix that can be seen as an operator on the range of $P^\perp = \mathbb{1} - P$. Moreover, it can be deduced that the first derivative acting again on $L^2(0, 1)^m$ with boundary conditions of the form

$$(L + P)\,(u(0) - u(1)) + P^\perp\,(u(0) + u(1)) = 0,$$

where P is an orthogonal projector in $\mathbb{C}^m$ and L a Hermitian operator acting in the range of $P^\perp$, generates a unitary group. This is due to the fact that by Stone's theorem, $i\frac{d}{dx}$ is then a self–adjoint operator on $L^2(0, 1)^m$. For $-L$ dissipative the above boundary conditions define m–dissipative realisations of the first derivative operator in $L^2(0, 1)^m$. This formal coincidence gives the starting point for this attempt to couple first and second derivatives by their boundary values.

An elementary integration by parts yields

$$\begin{aligned} \langle Au, v\rangle &= \int_{\mathcal{G}_d} \langle u_d'', v_d\rangle - \int_{\mathcal{G}_t} \langle u_t', v_t\rangle \\ &= -\int_{\mathcal{G}_d} \langle u_d', v_d'\rangle + [u_d', v_d]_{\partial\mathcal{I}_d} + \int_{\mathcal{G}_t} \langle u_t, v_t'\rangle - [u_t, v_t]_{\partial\mathcal{I}_t}, \end{aligned} \tag{40}$$

for $u, v \in \mathrm{Dom}(A)$, where here and in the following one denotes

$$\begin{aligned}
[u_d, v_d]_{\partial\mathcal{I}_d} &= \sum_{i=1}^{D} \left(u_{di}(a_{di})\overline{v}_{di}(a_{di}) - u_{di}(0)\overline{v}_{di}(0)\right), \\
[u_t, v_t]_{\partial\mathcal{I}_t} &= \sum_{j=1}^{T} \left(u_{ti}(a_{tj})\overline{v}_{tj}(a_{tj}) - u_{tj}(0)\overline{v}_{tj}(0)\right).
\end{aligned}$$

While the equation (40) is not particularly appealing, the real part of the associated quadratic form is

$$\text{(41)} \qquad \mathrm{Re}\,\langle Au, u\rangle = -\int_{\mathcal{G}_d} |u_d'|^2 + \mathrm{Re}\,[u_d', u_d]_{\partial\mathcal{I}_d} - \frac{1}{2}\,[u_t, u_t]_{\partial\mathcal{I}_t}\,, \qquad u \in \mathrm{Dom}(A).$$

For the sake of notational simplicity one introduces the finite dimensional auxiliary Hilbert space

$$\underline{\mathcal{K}} \equiv \underline{\mathcal{K}}(\mathcal{I}_d, \mathcal{I}_t) = \underline{\mathcal{K}}_{\mathcal{I}_d}^{-} \oplus \underline{\mathcal{K}}_{\mathcal{I}_d}^{+} \oplus \underline{\mathcal{K}}_{\mathcal{I}_t}$$

with $\underline{\mathcal{K}}_{\mathcal{I}_t} \cong \mathbb{C}^{|\mathcal{I}_t|}$ and $\underline{\mathcal{K}}_{\mathcal{I}}^{(\pm)} \cong \mathbb{C}^{|\mathcal{I}_d|}$. Define for any $u \in \mathcal{D}_d \oplus \mathcal{W}_t$ the two vectors of boundary values

$$\text{(42)} \quad \underline{u} := \begin{bmatrix} \{u_{di}(a_{di})\}_{1\le i\le D} \\ \{u_{di}(0)\}_{1\le i\le D} \\ 2^{-\frac{1}{2}}\{u_{tj}(a_{tj}) + u_{tj}(0)\}_{1\le j\le T} \end{bmatrix}, \qquad \underline{\underline{u}} := \begin{bmatrix} \{u_{di}'(a_{di})\}_{1\le i\le D} \\ \{-u_{di}'(0)\}_{1\le i\le D} \\ 2^{-\frac{1}{2}}\{-u_{tj}(a_{tj}) + u_{tj}(0)\}_{1\le j\le T} \end{bmatrix}$$

and note that $\underline{u}, \underline{\underline{u}} \in \underline{\mathcal{K}}$. With this notation equation (41) becomes well–arranged

$$\text{(43)} \qquad \mathrm{Re}\,\langle Au, u\rangle = -\int_{\mathcal{G}_d} |u_d'|^2 + \mathrm{Re}\,\langle \underline{\underline{u}}, \underline{u}\rangle_{\underline{\mathcal{K}}} \qquad \text{for all } u \in \mathrm{Dom}(A).$$

This formula motivates the introduction of boundary conditions of the form

$$\text{(44)} \qquad P^{\perp}\underline{\underline{u}} + (L + P)\underline{u} = 0,$$

where P is an orthogonal projector acting on $\underline{\mathcal{K}}$, $P^{\perp} = \mathbb{1} - P$ is its complementary projector, and L is an operator in $\mathrm{Ran}\,P^{\perp}$ (whose extension by 0 to the whole of $\underline{\mathcal{K}}$ is still denoted by L). The boundary conditions in equation (44) can be written equivalently as two separated conditions

$$P^{\perp}\underline{\underline{u}} + L\underline{u} = 0 \quad \text{and} \quad P\underline{u} = 0.$$

Inserting these boundary conditions in (43) delivers

$$\mathrm{Re}\,\langle Au, u\rangle = -\int_{\mathcal{G}_d} |u_d'|^2 - \mathrm{Re}\,\langle L\underline{u}, \underline{u}\rangle_{\underline{\mathcal{K}}}.$$

This leads to the definition of the operator $A_{P,L}$ given by

$$A_{P,L}u := Au, \quad u \in \mathrm{Dom}(A_{P,L}),$$

where

$$\text{(45)} \quad \mathrm{Dom}(A^0) \subset \mathrm{Dom}(A_{P,L}) = \{u \in \mathcal{D}_d \oplus \mathcal{W}_t \mid P^{\perp}\underline{\underline{u}} + (L + P)\underline{u} = 0\} \subset \mathrm{Dom}(A).$$

The boundary conditions can be expressed also by means of the *space of boundary values*

$$\underline{\mathcal{K}}^2 = \underline{\mathcal{K}} \oplus \underline{\mathcal{K}}$$

and the trace operator

$$[\cdot] : \mathcal{D}_d \oplus \mathcal{W}_t \to \underline{\mathcal{K}}^2, \quad u \mapsto [u] := \begin{bmatrix} \underline{u} \\ \underline{\underline{u}} \end{bmatrix}.$$

Observing that a function u satisfies the boundary conditions $(L+P)\underline{u} + P^{\perp}\underline{\underline{u}} = 0$ if and only if $[u] \in \operatorname{Ker}(L+P,\, P^{\perp})$, where

$$(L+P,\, P^{\perp})\colon\ \underline{\mathcal{K}} \oplus \underline{\mathcal{K}} \to \underline{\mathcal{K}}, \quad \begin{bmatrix} \underline{u} \\ \underline{\underline{u}} \end{bmatrix} \mapsto (L+P)\underline{u} + P^{\perp}\underline{\underline{u}},$$

one defines more generally for an arbitrary subspace $\mathcal{M} \subset \underline{\mathcal{K}}^2$ the operator $A_{\mathcal{M}}$ by

$$A_{\mathcal{M}} u := Au, \quad u \in \operatorname{Dom}(A_{\mathcal{M}}),$$

where

$$\operatorname{Dom}(A^0) \subset \operatorname{Dom}(A_{\mathcal{M}}) = \{(u_d, u_t) \in \mathcal{D}_d \oplus \mathcal{W}_t \mid [u] \in \mathcal{M}\} \subset \operatorname{Dom}(A).$$

Note that two boundary conditions define the same operator if and only if the corresponding subspaces in $\underline{\mathcal{K}}^2$ coincide. In this sense the operators P and L determine $A_{P,L}$ uniquely. All types of boundary conditions defining operators that lie between those with minimal and the maximal domain, can be parametrized in terms of subspaces of $\mathcal{M} \subset \underline{\mathcal{K}}^2$.

REMARK 3.2. *Considering concrete examples it often occurs that linear boundary conditions are given in terms of operators C and D, which act in $\underline{\mathcal{K}}$, and one considers $A_{\mathcal{M}}$ with*

$$\mathcal{M} = \mathcal{M}(C, D), \quad \textit{where } \mathcal{M}(C, D) = \operatorname{Ker}(C,\, D).$$

In this situation one can ask if there is an equivalent parametrization of the form (44)*. For this purpose one can use the scheme developed when studying quasi–m–accretive Laplacians in Chapter 1. Consider simultaneously the decompositions of $\underline{\mathcal{K}}$ with respect to* $\operatorname{Ker} D$*,* $(\operatorname{Ker} D)^{\perp}$ *and with respect to* $\operatorname{Ran} D$*,* $(\operatorname{Ran} D)^{\perp}$*. Here one denotes by Q the orthogonal projector onto* $(\operatorname{Ran} D)^{\perp}$*, $Q^{\perp} = \mathbb{1} - Q$ and by P the orthogonal projector onto* $\operatorname{Ker} D$*, $P^{\perp} = \mathbb{1} - P$. This induces a block structure on the map $(C,\, D)\colon \underline{\mathcal{K}}^2 \to \underline{\mathcal{K}}$,*

$$(C,\, D) = \begin{pmatrix} Q^{\perp}CP^{\perp} & Q^{\perp}CP & Q^{\perp}DP^{\perp} & 0 \\ QCP^{\perp} & QCP & 0 & 0 \end{pmatrix}.$$

This yields that the parametrization by $(C,\, D)$ is equivalent to certain $(L+P,\, P^{\perp})$ of the type (44) *whenever the map $(C,\, D)$ has maximal rank and $QCP^{\perp} \equiv 0$ holds. One observes that if $QCP^{\perp} \equiv 0$ holds, the block $Q^{\perp}CP$ does not play any role for the numerical range of $A_{\mathcal{M}}$. So, if the map $(C,\, D)$ has maximal rank and $QCP^{\perp} \equiv 0$ then equivalent boundary conditions are given by*

$$(C',\, D') = \begin{pmatrix} L & 0 & P^{\perp} & 0 \\ 0 & P & 0 & 0 \end{pmatrix},$$

where P denotes the orthogonal projector onto $\operatorname{Ker} D$ *and $L = (Q^{\perp}DP^{\perp})^{-1}Q^{\perp}CP^{\perp}$, compare also Remark 1.5 in Chapter 1.*

3.1.2. Quasi–m–dissipative operators. As already mentioned, the aim of this chapter is to discuss the parabolic properties of the abstract Cauchy problem associated with the operator $A_{P,L}$. The main result of this chapter is

THEOREM 3.3. *Let P be an orthogonal projector acting on $\mathcal{H}$ and L a linear operator on $\mathrm{Ker}P$ such that $-L$ satisfies the condition*

$$-\mathrm{Re}\,\langle Lx, x\rangle_{\underline{\mathcal{K}}} \leq \omega\left(|x_d^+|^2 + |x_d^-|^2\right) \qquad \text{for all } x := (x_d^+, x_d^-, x_t) \in \underline{\mathcal{K}} = \underline{\mathcal{K}}_d^+ \oplus \underline{\mathcal{K}}_d^- \oplus \underline{\mathcal{K}}_t \tag{46}$$

for some $\omega \geq 0$. Then the operator $A_{P,L}$ given by

$$A_{P,L}u = Au \quad \text{with } \mathrm{Dom}(A_{P,L}) = \{u \in \mathcal{D}_d \oplus \mathcal{W}_t \mid P^\perp \underline{\underline{u}} + (L+P)\underline{u} = 0\}$$

is quasi–m–dissipative, and in fact m-dissipative whenever $-L$ is dissipative. Accordingly, the operator $A_{P,L}$ is the infinitesimal generator of a quasi-contractive semigroup $(e^{tA_{P,L}})_{t\geq 0}$ on $\mathcal{H}$ and even a contractive semigroup if $-L$ is dissipative.

The above theorem yields in particular that the initial value problem

$$\begin{cases} \dfrac{\partial u}{\partial t}(t) &= A_{P,L}u(t), \qquad t \geq 0, \\ u(0) &= u_0 \in \mathcal{H}, \end{cases}$$

is well posed whenever $-L$ is dissipative or even satisfies (46), and the solution is given by

$$u(\cdot, t) := e^{tA_{P,L}}u_0, \qquad t \geq 0.$$

Furthermore, the question whether the solution $u(\cdot,t)$ is a real-valued function for all $t > 0$ if the initial data u_0 is real-valued can be answered in terms of the boundary conditions imposed at the vertices. This is discussed in the forthcoming Proposition 3.14. Before proving Theorem 3.3, two preparatory lemmata are needed.

LEMMA 3.4. *Let $\omega \geq 0$ be such that* (46) *is satisfied. Then $A_{P,L}$ is quasi-dissipative, and*

$$\mathrm{Re}\,\langle A_{P,L}u, u\rangle \leq -4\omega^2 \|u\|^2_{\mathcal{H}} \qquad \text{for all } u \in D(A_{P,L}). \tag{47}$$

If in particular $-L$ is dissipative, that is $\omega = 0$, then $A_{P,L}$ is dissipative.

PROOF. Take $u \in \mathrm{Dom}(A_{P,L})$, then from inserting $L\underline{u} + P^\perp \underline{\underline{u}} = 0$ and $P\underline{u} = 0$ in (43) it follows that

$$\mathrm{Re}\,\langle A_{P,L}u, u\rangle = -\|u'\|^2_{\mathcal{H}} + \mathrm{Re}\,\langle L\underline{u}, \underline{u}\rangle_{\underline{\mathcal{K}}}.$$

Let $\omega \geq 0$ be such that (46) is satisfied. Applying Lemma 1.13 to each edge one obtains with $l \leq a_{\min}$, where $a_{\min} := \min\{a_i \in \underline{a}\}$,

$$\begin{aligned} \mathrm{Re}\,\langle A_{P,L}u, u\rangle &= -\|u'\|^2_{\mathcal{H}} + \mathrm{Re}\,\langle L\underline{u}, \underline{u}\rangle_{\underline{\mathcal{K}}} \\ &\leq -\|u'\|^2_{\mathcal{H}} - \omega\|(u_d(a), u_d(0))\|^2 \\ &\leq -\|u'\|^2_{\mathcal{H}} - 2\omega\left(l\|u'\|^2_{\mathcal{H}} + \tfrac{2}{l}\|u\|^2_{\mathcal{H}}\right), \end{aligned} \tag{48}$$

and for $l \leq \frac{1}{2\omega}$

$$\mathrm{Re}\,\langle A_{P,L}u, u\rangle \quad \leq \quad -4\omega^2\|u\|^2_{\mathcal{H}}.$$

Note that if $-L$ is dissipative, then one is able to estimate just by

$$\mathrm{Re}\,\langle A_{P,L}u, u\rangle \leq -\|u'\|^2_{\mathcal{H}} \leq 0.$$

□

The Hilbert space adjoint of A^0 is the diagonal block operator matrix

$$B := \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & \frac{d}{dx} \end{bmatrix} \quad \text{with} \quad \mathrm{Dom}(B) := \mathcal{D}_d \oplus \mathcal{W}_t \subset \mathcal{H}.$$

The adjoint of the maximal operator A is the restriction of B to $\mathcal{D}_d^0 \oplus \mathcal{W}_t^0$, which is denoted by B^0, that is $B^0 = A^*$. Observe that $A_{P,L}$ is an extension of $A^0 = B^*$ and $A_{P,L}^*$ a restriction of B. Consequently one has the inclusions

$$A^0 \subset A_{P,L} \subset A \quad \text{and} \quad B^0 \subset A_{P,L}^* \subset B.$$

This allows to describe $A_{P,L}^*$ in terms of boundary conditions imposed on B. This is done analogously to the boundary conditions imposed on A. For this purpose introduce the adapted traces

$$\widetilde{v} = \begin{bmatrix} \{v_{di}(a_{di})\}_{1\le i\le D} \\ \{v_{di}(0)\}_{1\le i\le D} \\ 2^{-\frac{1}{2}}\{(v_{tj}(0) + v_{tj}(a_{tj}))\}_{1\le j\le T} \end{bmatrix}, \qquad \widetilde{\widetilde{v}} = \begin{bmatrix} \{v'_{di}(a_{di})\}_{1\le i\le D} \\ \{-v'_{di}(0)\}_{1\le i\le D} \\ 2^{-\frac{1}{2}}\{(-v_{tj}(0) + v_{tj}(a_{tj}))\}_{1\le j\le T} \end{bmatrix}$$

and observe that

$$\widetilde{v} = \underline{v}, \qquad \text{and} \qquad \widetilde{\widetilde{v}} = J\underline{\underline{v}}, \quad \text{where} \quad J := \begin{bmatrix} \mathbb{1}_{\underline{\mathcal{K}}_d^-} & 0 & 0 \\ 0 & \mathbb{1}_{\underline{\mathcal{K}}_d^+} & 0 \\ 0 & 0 & -\mathbb{1}_{\underline{\mathcal{K}}_t} \end{bmatrix}.$$

The change of sign from $\underline{\underline{v}}$ to $\widetilde{\widetilde{v}}$ in the last component is due to the change of the direction on the transport edges comparing A to B.

LEMMA 3.5. *The adjoint of $A_{P,L}$ is given by*

$$A_{P,L}^* v = Bv$$

with

$$\mathrm{Dom}(A_{P,L}^*) = \{(v_d, v_t) \in \mathcal{D}_d \oplus \mathcal{W}_t \mid (L^* + P)\widetilde{v} + P^\perp \widetilde{\widetilde{v}} = 0\}.$$

PROOF. By definition, the adjoint of $A_{P,L}$ is the operator defined on

$$\mathrm{Dom}(A_{P,L}^*) = \{v \in \mathcal{H} \mid \exists u \in \mathcal{H} \text{ with } \langle A_{P,L} w, v\rangle = \langle w, u\rangle \text{ for all } w \in \mathrm{Dom}(A_{P,L})\},$$

by $A_{P,L}^* v = u$, compare for example [92, Chapter 2.4]. To begin with, observe that an explicit calculation gives

$$\langle Au, v\rangle - \langle u, Bv\rangle = -\,\langle \underline{u}, \widetilde{\widetilde{v}}\rangle_{\underline{\mathcal{K}}} + \langle \underline{\underline{u}}, \widetilde{v}\rangle_{\underline{\mathcal{K}}}, \qquad \text{for } u, v \in \mathcal{D}_d \oplus \mathcal{W}_t,$$

or rather

$$\langle Au, v\rangle - \langle u, Bv\rangle = \left\langle \begin{bmatrix} \underline{u} \\ \underline{\underline{u}} \end{bmatrix}, \begin{bmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{bmatrix} \begin{bmatrix} \underline{v} \\ J\underline{\underline{v}} \end{bmatrix} \right\rangle_{\underline{\mathcal{K}}^2}, \tag{49}$$

where $u, v \in \mathcal{D}_d \oplus \mathcal{W}_t$. Recall that $A_{P,L}^*$ is a restriction of the operator B. Hence $v \in \mathrm{Dom}(A_{P,L}^*)$ if and only if the boundary term in (49) vanishes for all $u \in \mathrm{Dom}(A_{P,L})$. The range of

$$[\cdot]_{P,L} \colon \mathrm{Dom}(A_{P,L}) \to \underline{\mathcal{K}}^2, \quad [u]_{P,L} = [u]$$

is $\operatorname{Ker}(L + P,\, P^{\perp})$. Consequently the boundary term (49) vanishes for a fixed $v \in \mathcal{D}_d \oplus \mathcal{W}_t$ and all $u \in \operatorname{Dom}(A_{P,L})$ if and only if

$$\begin{bmatrix} \underline{v} \\ J\underline{\underline{v}} \end{bmatrix} \quad \text{is orthogonal to} \quad \begin{bmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{bmatrix} \operatorname{Ker}\left(L + P,\, P^{\perp}\right).$$

The orthogonal complement of the space

$$\begin{bmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{bmatrix} \operatorname{Ker}(L + P,\, P^{\perp}) = \operatorname{Ker}(-P^{\perp},\, L + P)$$

is exactly $\operatorname{Ker}(L^* + P,\, P^{\perp})$. One summarizes that $v \in \operatorname{Dom}(A^*_{P,L})$ if and only if $v \in \mathcal{D}_d \oplus \mathcal{W}_t$ and

$$\begin{bmatrix} \underline{v} \\ J\underline{\underline{v}} \end{bmatrix} = \begin{bmatrix} \widetilde{v} \\ \widetilde{\widetilde{v}} \end{bmatrix} \in \operatorname{Ker}(L^* + P,\, P^{\perp})$$

holds. This completes the proof. □

PROOF OF THEOREM 3.3. A sufficient condition for a densely defined operator to have m–dissipative closure is that both the operator and its adjoint are dissipative, see [33, Corollary II.3.17]. By Lemma 3.4, the operator $A_{P,L}$ is quasi–dissipative for any L satisfying (46) for some $\omega \geq 0$ and dissipative whenever $-L$ is dissipative. Analogous to Lemma 3.4 one can prove that conversely the operator $A^*_{P,L}$ is quasi–dissipative for any L satisfying (46) for some $\omega \geq 0$, and dissipative whenever $-L$ is dissipative using

$$\operatorname{Re}\langle Bu, u\rangle = -\int_{\mathcal{G}_d} |u_d'|^2 + \operatorname{Re}\langle \widetilde{\widetilde{u}}, \widetilde{u}\rangle_{\underline{\mathcal{K}}}, \qquad u \in \mathcal{D}_d \oplus \mathcal{W}_t.$$

To conclude the proof it suffices to check that $A_{P,L}$ is actually closed. As both the first and the second derivative without boundary conditions are closed operators, here it suffices to check that the boundary conditions are respected in the limit. This follows from the fact that the trace operators $u \mapsto \underline{u}$ and $u \mapsto \underline{\underline{u}}$ considered as operators from the Hilbert space $\mathcal{D}_d \oplus \mathcal{W}_t$ to $\underline{\mathcal{K}}$ are bounded. □

REMARK 3.6. *Observe that dissipativity of the matrix $-L$ is sufficient but not necessary for $A_{P,L}$ to be m–dissipative. This is shown by means of an example.*

Consider the graph consisting of one transport and one diffusion edge with certain lengths a_d and a_t, and boundary conditions as in (44) *by taking*

$$P := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \textit{and} \quad L_\alpha := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -\sqrt{2}\alpha & 1 \end{bmatrix}, \quad \alpha > 0.$$

This corresponds to the boundary conditions

$$u_d(a_t) = 0, \qquad u_d'(0) = 0, \quad \textit{and} \quad \alpha\, u_d(0) = u_t(0).$$

Inserting this into (41) *delivers*

$$\operatorname{Re}\langle A_{P,L_\alpha} u, u\rangle = -\int_{\mathcal{G}_d} |u_d'|^2 - \frac{1}{2}|u_t(a_t)|^2 + \frac{\alpha^2}{2}|u_d(0)|^2, \quad u \in \operatorname{Dom}(A_{P,L_\alpha}).$$

Note that the form defined by

$$-\int_{\mathcal{G}_d} |u_d'|^2 + \frac{\alpha^2}{2}|u_d(0)|^2, \quad u \in \{\mathcal{W}_d \mid u_d(a_d) = 0\}$$

is dissipative for $\alpha > 0$ small enough. By Proposition 2.15 in Chapter 2 for $\{\mathcal{W}_d \mid u_d(a_d) = 0\}$ a Poincaré type inequality $\|u\|_{\mathcal{H}} \leq C\|u_d'\|_{\mathcal{H}}$ holds for a constant $C > 0$,

$$|u_d(0)|^2 \leq C'\|u_d'\|^2,$$

for a constant $C' > 0$. Hence one obtains by Lemma 1.13

$$\operatorname{Re}\langle A_{P,L_\alpha}u, u\rangle \leq 0, \quad \textit{for } \left(\frac{\alpha^2}{2}C' - 1\right) \leq 0,$$

that is A_{P,L_α} is dissipative even if the operator $-L_\alpha$ is not. Since L_α satisfies (46) for some $\omega > 0$ for $\alpha > 0$ small enough one has by theorem 3.3 that the operator A_{P,L_α} is m–dissipative for $\alpha > 0$ small, although L_α was not.

Note that Theorem 3.3 does not contain a characterization of not all quasi–m–dissipative extensions of A^0. However, it seems likely that the class of extensions discussed here covers all.

3.2. Spectral theory

Taking into account the compact embedding of $\mathcal{W}$ into $\mathcal{H}$, compare for example [4, Theorem A. 5.4], one promptly obtains the following

LEMMA 3.7. *For all orthogonal projectors P on $\underline{\mathcal{K}}$ and all linear operators L acting on $\operatorname{Ker}P$ satisfying (46) the operators $A_{P,L}$ have compact resolvents. In particular, the operators $A_{P,L}$ have only pure point spectrum.*

3.2.1. Non–zero eigenvalues. In order to determine the non–zero pure point spectrum of $A_{P,L}$, a natural *Ansatz* for finding eigenfunctions is to take $k \in \mathbb{C} \setminus \{0\}$ and to consider

$$\phi(x,k) = \begin{cases} \alpha_{di}(k)e^{ikx} + \beta_{di}(k)e^{-ikx}, & x \in \mathsf{e}_{di},\ i = 1,\dots,D, \\ \gamma_{tj}(k)e^{k^2x}, & x \in \mathsf{e}_{tj},\ j = 1,\dots,T. \end{cases}$$

The boundary conditions $(P + L)\underline{\phi(\cdot,k)} + P^\perp\underline{\underline{\phi(\cdot,k)}} = 0$ are encoded in

$$[(P + L)\underline{X}(k) + P^\perp\underline{Y}(k)]\begin{bmatrix}\alpha_d(k)\\ \beta_d(k)\\ \gamma_t(k)\end{bmatrix} = 0,$$

where $\alpha_d(k)$, $\beta_d(k)$ and $\gamma_t(k)$ are the vectors with the sought after coefficients with entries

$$\{\alpha_d(k)\}_i = \alpha_{di}(k), \quad \{\beta_d(k)\}_i = \beta_{di}(k) \text{ and } \{\gamma_t(k)\}_j = \gamma_{tj}(k).$$

Furthermore one has used the matrices

$$\underline{X}(k) = \begin{bmatrix} e^{ik\underline{a}_d} & e^{-ik\underline{a}_d} & 0 \\ \mathbb{1} & \mathbb{1} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}(\mathbb{1} + e^{k^2\underline{a}_t}) \end{bmatrix} \text{ and}$$

$$\underline{Y}(k) = \begin{bmatrix} ike^{ik\underline{a}_d} & -ike^{-ik\underline{a}_d} & 0 \\ -ik & ik & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}(\mathbb{1} - e^{k^2\underline{a}_t}) \end{bmatrix},$$

which are given with respect to the decomposition $\underline{\mathcal{K}} = \underline{\mathcal{K}}^+_{\mathcal{I}_d} \oplus \underline{\mathcal{K}}^-_{\mathcal{I}_d} \oplus \underline{\mathcal{K}}_{\mathcal{I}_t}$. Accordingly, the following characterization of the eigenvalues holds.

PROPOSITION 3.8. *The number $-k^2 \in \mathbb{C} \setminus \{0\}$ is an eigenvalue of $A_{P,L}$ if and only if the matrix*

$$\underline{Z}_{P,L}(k) := [(P+L)\underline{X}(k) + P^{\perp}\underline{Y}(k)]$$

has non trivial null space. The geometric multiplicity of $-k^2$ equals the dimension of the space $\mathrm{Ker}\underline{Z}_{P,L}(k)$.

Hence, the secular equation for the operator $A_{P,L}$ for any projector P and operator L acting in $\mathrm{Ker}\, P$ is

$$\det \underline{Z}_{P,L}(k) = 0.$$

EXAMPLE 3.9. *Consider the graph consisting of one diffusion edge of length a_d and one transport edge of length a_t. Let P be as in Remark 3.6,*

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2^{-1} & 2^{-1} \\ 0 & 2^{-1} & 2^{-1} \end{bmatrix} \quad \textit{and} \quad L = 0.$$

Then the operator $A_{P,L}$ is m–dissipative and the secular equation becomes

$$\det \underline{Z}_{P,L}(k) = \frac{i}{\sqrt{2}} \left[\sin(ka_d) \left(1 - e^{k^2 a_t}\right) + k\cos(ka_d)\left(1 + e^{k^2 a_t}\right)\right] = 0.$$

In particular the spectrum of $A_{P,L}$ contains a sequence of real eigenvalues going to $-\infty$.

In general it seems to be a difficult task giving precise statements on the distribution of the eigenvalues.

3.2.2. Eigenvalue zero. For the eigenvalue zero one uses the *Ansatz*

$$\phi^0(x) = \begin{cases} \alpha^0_{di} + \beta^0_{di} x, & x \in \mathsf{e}_{di},\ i = 1, \dots, D, \\ \gamma^0_{tj}, & x \in \mathsf{e}_{tj},\ j = 1, \dots, T. \end{cases}$$

The boundary conditions $(P+L)\underline{\phi^0(\cdot)} + P^{\perp}\underline{\underline{\phi^0(\cdot)}} = 0$ are encoded in

$$[(L+P)\underline{X}^0 + P^{\perp}\underline{Y}^0] \begin{bmatrix} \alpha^0_d \\ \beta^0_d \\ \gamma^0_t \end{bmatrix} = 0$$

with

$$\underline{X}^0 = \begin{bmatrix} \mathbb{1} & \underline{a}_d & 0 \\ \mathbb{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \quad \text{and} \quad \underline{Y}^0 = \begin{bmatrix} 0 & \mathbb{1} & 0 \\ 0 & -\mathbb{1} & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

This gives a characterization for the eigenvalue zero.

PROPOSITION 3.10. *The operator $A_{P,L}$ has eigenvalue zero if and only if*

$$\det \underline{Z}^0_{P,L} = 0, \quad \textit{where} \quad \underline{Z}^0_{P,L} = (P+L)\underline{X}^0 + P^{\perp}\underline{Y}^0.$$

In particular, the invertibility of the operator $A_{P,L}$ for L satisfying (46) is independent of the lengths of the transport edges. This is due to the fact that elements of the kernel are constant on the transport edges.

EXAMPLE 3.11. *Consider again the graph given in Example 3.9 and let P be the projector given in Example 3.9 and Remark 3.6. Let be $L_C = CP^{\perp}$, where $P^{\perp} = \mathbb{1} - P$ and for arbitrary $C \in \mathbb{C}$. Then*

$$\det \underline{Z}^0_{P,L_C} = -2^{-\frac{1}{2}} - Ca_D 2^{-\frac{1}{2}}$$

and therefore A_{P,L_C} is invertible only for $C \neq -(2a_D)^{-1}$.

3.2.3. The resolvent operator. For $A_{P,L}$ quasi–m–dissipative, knowing the resolvent, one can describe the strongly continuous semigroup generated by $A_{P,L}$ in terms of the inverse Laplace transform as

$$e^{tA_{P,L}}u = \lim_{n\to\infty} \int_{\varepsilon-in}^{\varepsilon+in} e^{t\lambda} \left(A_{P,L} - \lambda\right)^{-1} u \, d\lambda, \qquad u \in \mathcal{H}, \tag{50}$$

for any $\varepsilon > \omega$ if $A_{P,L} + \omega$ is dissipative, see [5, Theorem 3.12.2] or [79, Corollary 7.5]. In the following an explicit formula for the resolvent is given in terms of the boundary conditions and the edge lengths. The notion of *integral operators* is going to be made precise in the forthcoming Definition 4.25.

PROPOSITION 3.12. *For all $k \in \mathbb{C} \setminus \{0\}$ with $\operatorname{Im} k > 0$ such that $-k^2 \in \rho(A_{P,L})$ the resolvent*

$$R(k^2) = (A_{P,L} + k^2)^{-1}$$

is the integral operator defined by

$$R(k^2)u(x) = \int_{\mathcal{G}} \underline{r}(x, y, k)u(y)dy$$

with kernel

$$r(x, y, k) = \left[r_0(x, y, k) - \underline{\Phi}(x, k)\underline{\Sigma}_{P,L}(k)\underline{\Psi}(y, k)\right] \underline{W}(k).$$

Here one has set

$$\underline{\Sigma}_{P,L}(k) = [(P + L)\underline{X}(k) + P^{\perp}\underline{Y}(k)]^{-1}[P^{\perp}\underline{R}_1(k) + (L + P)\underline{R}_2(k)]$$

and furthermore

$$\begin{aligned} r_0(x, y, k) &= \begin{bmatrix} r_d(x, y, k) & 0 \\ 0 & r_t(x, y, k^2) \end{bmatrix}, \\ \underline{W}(k) &= \begin{bmatrix} \frac{i}{2k}\mathbb{1} & 0 \\ 0 & \mathbb{1} \end{bmatrix}, \end{aligned}$$

where $r_d(x, y, k)$ is an $|\mathcal{I}_d| \times |\mathcal{I}_d|$–diagonal matrix with entries

$$\{r_d(x, y, k)\}_{n,m} = \delta_{n,m} e^{ik|x-y|}$$

and $r_t(x, y, k)$ is an $|\mathcal{I}_t| \times |\mathcal{I}_t|$–diagonal matrix with entries

$$\{r_t(x, y, k)\}_{n,m} = \delta_{n,m} \left(\begin{cases} e^{k^2(x-y)}, & x < y \\ 0, & x \geq y \end{cases} \right).$$

Finally,

$$\underline{\Phi}(x, k) = \begin{bmatrix} e^{ikx} & e^{-ikx} & 0 \\ 0 & 0 & e^{k^2x} \end{bmatrix}, \qquad \underline{\Psi}(y, k) = \begin{bmatrix} e^{iky} & 0 \\ e^{-iky} & 0 \\ 0 & e^{-k^2y} \end{bmatrix},$$

where the entries are diagonal matrices the entries of which are functions with arguments from the corresponding edges and

$$\underline{R}_1(k) = \begin{bmatrix} ik\mathbb{1} & 0 & 0 \\ 0 & ike^{ik\underline{a}_d} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}\mathbb{1} \end{bmatrix}, \qquad \underline{R}_2(k) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & e^{ik\underline{a}_d} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}\mathbb{1} \end{bmatrix}.$$

COROLLARY 3.13. *For $-k^2 \in \rho(A_{P,L})$ the resolvents $(A_{P,L} + k^2)^{-1}$ are of p-th Schatten class for all $p > 1$ and, in particular, of Hilbert–Schmidt class.*

PROOF. For $-k^2 \in \rho(A_{P,L})$ the resolvents $(A_{P,L} + k^2)^{-1}$ are compact by Lemma 3.7. Furthermore, the operator $A_{\mathbb{1},0}$ satisfies the assumptions of Theorem 3.3, and therefore there exists a $0 > -C \in \rho(A_{P,L}) \cap \rho(A_{\mathbb{1},0})$. By Proposition 3.12 the difference

$$(A_{P,L} + C)^{-1} - (A_{\mathbb{1},0} + C)^{-1}$$

is a finite rank operator. Since the operator $(A_{\mathbb{1},0} + C)^{-1}$ is of p-th Schatten class for all $p > 1$ the claim follows. $\square$

PROPOSITION 3.14. *Provided that L and P have real entries, and L satisfies* (46). *Then the semigroup $(e^{tA_{P,L}})_{t\geq 0}$ generated by $A_{P,L}$ is real.*

PROOF. The kernel $r(\cdot, \cdot, i\kappa)$ has real coefficients whenever the operators L and P have real entries. Therefore the resolvents $(A_{P,L} - \lambda)^{-1}$ map real valued functions in $\mathcal{H}$ to real valued functions for any $\lambda > 0$ with $\lambda \in \rho(A_{P,L})$. Applying the inverse Laplace transform (50) one concludes that the semigroup generated by $A_{P,L}$, $e^{tA_{P,L}}$ is real, whenever P and L are real. $\square$

PROOF OF PROPOSITION 3.12. It is sufficient to prove that $r(x, y, k)$ is the Green's function for the problem. Consider the unperturbed operator

$$R^0(k^2)u = \int_{\mathcal{G}} r_0(x, y, k)\underline{W}(k)u(y)dy \qquad \text{for } u \in \mathcal{D}',$$

where

$$\mathcal{D}' = \left(\bigoplus_{i=1}^{D} C_0^\infty([0, a_{di}]; \mathbb{C}) \bigoplus_{j=1}^{T} C_0^\infty([0, a_{tj}]; \mathbb{C}) \right).$$

The equation $(A+k^2)R^0(k^2)u = u$ is satisfied on the diffusion edges, because $\frac{i}{2k}e^{ik|x-y|}$ is the Green's function of $L_d(k) = \frac{d^2}{dx^2} + k^2$ on the whole real line (this follows from standard arguments using the Fourier transform). By continuing functions $u_i \in C_0^\infty([0, a_{di}]; \mathbb{C})$ trivially to the real line the claim follows. Similarly the diagonal entries of $r_t(x, y, k)$ are the Green's function for $L_t(k) = -\frac{d}{dx} + k^2$ on the whole real line, which follows from standard arguments from the theory of ordinary differential equations. Again by continuing functions u_j in $C_0^\infty([0, a_{tj}]; \mathbb{C})$ trivially to the real line the claim follows. Hence $(A + k^2)R^0(k^2)u = u$ holds for all $u \in \mathcal{D}'$.

For the correction term one has

$$(A + k^2) \int_{\mathcal{G}} \underline{\Phi}(x, k)\underline{\Sigma}_{P,L}(k)\underline{\Psi}(y, k)u(y)dy = 0.$$

Therefore $(A + k^2)R(k^2)u = u$, for any $u \in \mathcal{D}'$. Since $\mathcal{D}'$ is dense in $\mathcal{H}$ and $r(\cdot, \cdot, k)$ defines for all $k \neq 0$ with $k \in \rho(A_{P,L})$ a bounded linear operator on the square integrable functions, one concludes by density that $(A + k^2)R(k^2)u = u$ for all $u \in \mathcal{H}$.

It remains to prove that

$$R(k^2)u = \int_{\mathcal{G}} r(\cdot, y, k)u(y)dy \in \mathrm{Dom}(A_{P,L}).$$

Observe that for all $a > 0$ and all $u \in L^2([0, a]; \mathbb{C})$

$$\begin{aligned}
\left[\int_0^a e^{ik|x-y|}u(y)dy\right]_{x=0} &= \int_0^a e^{iky}u(y)dy, \\
\left[\int_0^a e^{ik|x-y|}u(y)dy\right]_{x=a} &= e^{ika}\int_0^a e^{-iky}u(y)dy, \\
\left[-\frac{d}{dx}\int_0^a e^{ik|x-y|}u(y)dy\right]_{x=0} &= ik\int_0^a e^{iky}u(y)dy, \\
\left[\frac{d}{dx}\int_0^a e^{ik|x-y|}u(y)dy\right]_{x=a} &= ike^{ika}\int_0^a e^{-iky}u(y)dy,
\end{aligned}$$

and considering only the edge $[0, a]$

$$\begin{aligned}
\left[\int_0^a r_t(x, y, k^2)u(y)dy\right]_{x=0} &= \int_0^a e^{-k^2 y}f(y)dy, \\
\left[\int_0^a r_t(x, y, k^2)u(y)dy\right]_{x=a} &= 0.
\end{aligned}$$

This gives in the matrix notation for $u \in \mathcal{H}$ and $v \in \underline{\mathcal{K}}$

$$\begin{aligned}
\underline{R^0(k^2)u(x)} &= \underline{R}_2(k)\int_{\mathcal{G}} \underline{\Psi}(k, y)\underline{W}(k)u(y)dy, &\qquad \underline{\Phi(x, k)v} &= \underline{X}(k)v, \\
\underline{\underline{R^0(k^2)u(x)}} &= \underline{R}_1(k)\int_{\mathcal{G}} \underline{\Psi}(k, y)\underline{W}(k)u(y)dy, &\qquad \underline{\underline{\Phi(x, k)v}} &= \underline{Y}(k)v.
\end{aligned}$$

Therefore

$$\begin{aligned}
\underline{\int_{\mathcal{G}} r(x, y, k)u(y)dy} &= (\underline{R}_2(k) - \underline{X}(k)\underline{\Sigma}_{P,L}(k))\int_{\mathcal{G}} \underline{\Psi}(y, k)\underline{W}(k)u(y)dy, \\
\underline{\underline{\int_{\mathcal{G}} r(x, y, k)u(y)dy}} &= (\underline{R}_1(k) - \underline{Y}(k)\underline{\Sigma}_{P,L}(k))\int_{\mathcal{G}} \underline{\Psi}(y, k)\underline{W}(k)u(y)dy,
\end{aligned}$$

and hence for all $u \in \mathcal{H}$

$$(P + L)\underline{\underline{\int_{\mathcal{G}} r(x, y, k)f(y)dy}} + P^{\perp}\underline{\int_{\mathcal{G}} r(x, y, k)f(y)dy} = 0.$$

This proves that $r(x, y, k)$ is the Green's function for the mixed problem. As it defines additionally a bounded integral operator in $\mathcal{H}$ one concludes that it is the resolvent's kernel. $\square$

3.3. A simplified model of a dendro–dendritical synapse

A possible application of the theory presented here are delayed diffusion equations. It is a classical idea, thoroughly developed for example in [10], that delays can mathematically be modelled by means of auxiliary transport phenomena.

To be more illustrative a model of a dendro–dendritical chemical synapse is discussed in this section. This model has been developed by Delio Mugnolo and Stefano Cardanobile as a very simplified model of a dendro–dendritical synapse, the dynamics of which are governed by a strongly continuous semigroup and it is included in [54]. For basic notions and miscellaneous models the reader is referred to the introductory textbook on neuronal modelling, [84, Chapters 2 and 9]. Actually, this simplified model has been the starting point for this work on more general diffusion and transport systems on compact metric graphs and it is presented here now as an application of the theory developed in this chapter. Of course, although the situation considered here is motivated by a simplified neuronal model, it can also be regarded as a simple example of a general diffusion equation with boundary delays.

Consider two dendrites, each modelled by an edge of length one e_1 and e_2, respectively. These are incident in the synapse $\mathsf{v}_{del} = \partial^+(\mathsf{e}_1) = \partial^-(\mathsf{e}_2)$, which is terminal endpoint of e_1 and initial endpoint of e_2. The synaptic input coming from e_1 undergoes a time–delay of $\tau_{\mathrm{del}} = 1$ before reaching e_2 and cannot double back. For the sake of simplicity, impose *sealed end* conditions on the first dendrite e_1 as well as on the second endpoint of e_2.

The synaptic input is an action potential that lets neurotransmitters be released by synaptic vesicles. It seems that no obvious biological connection exists between the unknowns u_1, u_2 in the diffusion equations corresponding to diffusion of pre- and post-synaptic potential in the dendrites. The unknown u_{del} in the equation models the transport of neurotransmitters between u_1, u_2. This system is proposed by a network diffusion problem with boundary delay

$$\text{(BD)} \qquad \begin{cases} \dot{u}_1(t,x) &=& u_1''(t,x), & t \geq 0,\ x \in (0,1), \\ \dot{u}_2(t,x) &=& u_2''(t,x), & t \geq 0,\ x \in (0,1), \\ u_1(t,1) &=& -\gamma^{-1} u_1'(t,1), & t \geq 0, \\ u_2(t,0) &=& \delta^{-1}\left(u_2'(t,0) + u_1(t-1,1)\right), & t \geq 0, \\ u_1'(t,0) &=& 0, & t \geq 0, \\ u_2'(t,1) &=& 0, & t \geq 0, \\ u_1(0,x) &=& f_1(0,x), & x \in (0,1), \\ u_2(0,x) &=& f_2(0,x), & x \in (0,1), \\ u_1(t,1) &=& f_{\mathrm{del}}(t), & t \in [-1,0]. \end{cases}$$

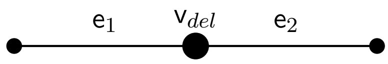
The first boundary condition can be interpreted by saying that a certain fraction γ^{-1} of all ions reaching the presynaptic nerve terminal is reflected into the dendrite – another amount δ^{-1}, actually flows further, thus forcing the vesicles to release into the synaptic cleft the neurotransmitters they contain. Finally, one observes that the above problem is undetermined if the last initial condition on the delay term is not imposed.

In order to implement the delay feature into the node conditions, the usual continuity assumptions are modified and one imposes the condition that the presynaptic potential at time t satisfies the continuity condition

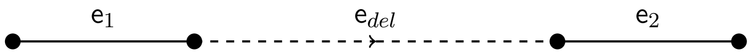
$$u_1(t,1) = u_{\mathrm{del}}(t,0), \qquad t \geq 0.$$

The aim is now to replace the fourth, delayed equation in (BD) by two node conditions in the endpoints of $\mathsf{e}_{\mathrm{del}}$. More precisely

$$u_2'(t,0) = \delta u_2(t,0) - u_{\mathrm{del}}(t,1), \qquad t \geq 0. \tag{51}$$



(a) Model with time–delay vertex.



(b) Equivalent model with auxiliary transport edge

FIGURE 2. Diffusion with time delay modelled by inserting an auxiliary transport edge.

This equation means that all neurotransmitters reaching the opposite side of the synaptic gap, as well as δ–times the ions sitting in the postsynaptic nerve terminal, determine the flow of *postsynaptic potential*. In other words, one is led to consider an (undelayed) initial boundary value problem

$$
(\mathrm{BD}') \qquad \left\{\begin{array}{rcll}
\dot u_1(t,x) &=& u_1''(t,x), & t\geq 0,\ x\in(0,1),\\
\dot u_{\mathrm{del}}(t,x) &=& -u_{\mathrm{del}}'(t,x), & t\geq 0,\ x\in(0,1),\\
\dot u_2(t,x) &=& u_2''(t,x), & t\geq 0,\ x\in(0,1),\\
u_1(t,1) &=& u_{\mathrm{del}}(t,0), & t\geq 0,\\
u_1'(t,1) &=& -\gamma u_1(t,1), & t\geq 0,\\
u_2'(t,0) &=& \delta u_2(t,0)-u_{\mathrm{del}}(t,1), & t\geq 0,\\
u_1'(t,0) &=& 0, & t\geq 0,\\
u_2'(t,1) &=& 0, & t\geq 0,\\
u_1(0,x) &=& f_1(0,x), & x\in(0,1),\\
u_2(0,x) &=& f_2(0,x), & x\in(0,1),\\
u_{\mathrm{del}}(0,x) &=& f_{\mathrm{del}}(0,x), & x\in(0,1).
\end{array}\right.
$$

Thus one has got rid of the boundary delay by passing to a larger state space. Observe that the above model is intrinsically non–symmetric in the sense that potential can only flow from dendrite e_1 to e_2, but not vice versa. This is a typical feature of *chemical synapses*, as opposed to *electric* ones. In particular taking the limit of the transport edge's length to zero the features of the model cannot move towards those of a purely diffusive model. One can check that the problems (BD) and (BD') are equivalent.

It should be observed that transport–based synaptic transmission models are not very common in literature. Due to their numerical and analytic complexity they are actually often replaced by convective–diffusive (or even purely diffusive) models. A convincing pleading of a transport approach can be found in [95, § 2 and § 6].

To discuss the problems (BD) and (BD') in the setting provided in Section 3.1, observe that (BD') can be seen as an abstract Cauchy problem on the Hilbert space $\mathcal{H}$ defined on the metric graph $(\mathcal{G},\underline{a})$, where $|\mathcal{I}_d|=2$ and $|\mathcal{I}_t|=1$, and each edge has length one. The corresponding spatial differential operator is $A_{P,L}$ with

$$L_{\gamma,\delta} = \begin{bmatrix} \gamma & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & \delta & -\sqrt{2} \\ \sqrt{2} & 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad P = 0.$$

Since

$$\operatorname{Re} L = \frac{1}{2}(L + L^*) \quad = \quad \frac{1}{2} \begin{bmatrix} 2\gamma & 0 & 0 & -1 & \sqrt{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 2\delta & -\sqrt{2} \\ \sqrt{2} & 0 & 0 & -\sqrt{2} & 2 \end{bmatrix}$$

is not sign definite for all $\gamma, \delta \in \mathbb{R}$, the matrix $-L$ is not dissipative for all $\gamma, \delta \in \mathbb{R}$. However, one has

$$\begin{aligned} &- \langle \operatorname{Re} Lx, x \rangle = \\ &- \gamma |x_{d1}^+|^2 - \delta |x_{d2}^-|^2 - |x_t|^2 \\ &- \frac{1}{2} \left\langle \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} x_{d1}^+ \\ x_{d2}^- \end{bmatrix}, \begin{bmatrix} x_{d1}^+ \\ x_{d2}^- \end{bmatrix} \right\rangle - \frac{1}{2} \left\langle \begin{bmatrix} 0 & 0 & \sqrt{2} \\ 0 & 0 & -\sqrt{2} \\ \sqrt{2} & -\sqrt{2} & 0 \end{bmatrix} \begin{bmatrix} x_{d1}^+ \\ x_{d2}^- \\ x_t \end{bmatrix}, \begin{bmatrix} x_{d1}^+ \\ x_{d2}^- \\ x_t \end{bmatrix} \right\rangle . \end{aligned}$$

Decomposing the matrix as above is critic, as this allows to find norms

$$\omega_1 := \left\| \frac{1}{2} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \right\| = \frac{1}{2} \quad \text{and} \quad \omega_2 := \left\| \frac{1}{2} \begin{bmatrix} 0 & 0 & \sqrt{2} \\ 0 & 0 & -\sqrt{2} \\ \sqrt{2} & -\sqrt{2} & 0 \end{bmatrix} \right\| = 1,$$

and subsequently to estimate

$$-\langle \operatorname{Re} Lx, x \rangle \leq (\omega_1 + \omega_2 - \operatorname{Re} \gamma)\, |x_{d1}^+|^2 + (\omega_1 + \omega_2 - \operatorname{Re} \delta)\, |x_{d2}^-|^2 + (\omega_2 - 1)|x_t|^2,$$

whence

$$-\langle \operatorname{Re} Lx, x \rangle \leq \left(\frac{3}{2} + \max\{-\operatorname{Re} \gamma, -\operatorname{Re} \delta\} \right) \left(|x_d^+|^2 + |x_d^-|^2 \right).$$

This shows that (46) is satisfied and a direct application of Theorem 3.3 yields finally the following

REMARK 3.15. *The initial-boundary value problem* (BD′) *is governed by a strongly continuous semigroup* $(T(t))_{t\geq 0}$ *on* $\mathcal{H} = L^2(0,1) \oplus L^2(0,1) \oplus L^2(0,1)$. *By Proposition 3.14 the semigroup generated by* $A_{P,L_{\gamma,\delta}}$ *is always real. This reflects the fact that all quantities involved in the model, like the action potentials, are naturally real quantities. Explicit computations show that*

$$\det \underline{Z}_{P,L}^0 = \sqrt{2}\delta\gamma$$

and therefore $A_{P,L_{\gamma,\delta}}$ *is invertible for all edge lengths as long as* $\gamma, \delta \neq 0$. *Considering* $\gamma = \delta = \frac{1}{2}$, *one obtains that* $\operatorname{Re} - L_{\gamma,\delta}$ *has the eigenvalues* 0 *and* -2. *Hence* $-L_{\gamma,\delta}$ *is dissipative for this particular case. Consequently* $A_{P,L_{\gamma,\delta}}$ *is m–dissipative for* $\gamma = \delta = \frac{1}{2}$ *by Theorem 3.3* *and in turn it generates a strongly continuous contractive semigroup, which describes the time–evolution of the system* (BD′).

REMARK 3.16. *Let for simplicity be $\gamma = \delta = 0$. Then the boundary conditions in* (BD′) *read*

$$\begin{array}{rcll} u_1(t,1) &=& u_{\mathrm{del}}(t,0), & t \geq 0, \\ u_1'(t,1) &=& 0, & t \geq 0, \\ u_2'(t,0) &=& -u_{\mathrm{del}}(t,1), & t \geq 0, \end{array}$$

which can be seen as transmission of the boundary values and of the flow on the left and on the right endpoints of $\mathsf{e}_{\mathrm{del}}$*, respectively; complemented by a Neumann boundary condition on the left endpoint. One concludes by observing that – dually, in a certain sense – one could have imposed transmission of the flow and of the boundary values on the left and on the right endpoints of* $\mathsf{e}_{\mathrm{del}}$*, respectively; again complemented by a Neumann boundary condition on the right endpoint. This can be discussed in a similar way. Another, perhaps more natural possibility would be to impose transmission of either boundary values at both endpoints, or transmission of flow at both endpoints. It seems that these two possibilities are not covered by the setting provided in Section 3.1 and it is not clear if this is a hint that such systems are not well–posed.*

3.4. Further examples of mixed dynamics

The study of mixed dynamics is a new aspect in the theory of differential equations on networks, and in the following further examples are discussed briefly.

3.4.1. Momentum and Laplace operators. Instead of considering the Cauchy problem with m–dissipative operators one might think of a Cauchy problem of Schrödinger type involving self–adjoint operators with mixed dynamics. To this aim let $(\mathcal{G}, \underline{a})$ be a compact metric graph with the subdivision $\mathcal{I} = \mathcal{I}_d \dot{\cup} \mathcal{I}_t$. Consider the closed symmetric operator

$$S^0 := \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & i\frac{d}{dx} \end{bmatrix} \quad \text{with} \quad \mathrm{Dom}(S^0) := \mathcal{D}_d^0 \oplus \mathcal{W}_t^0.$$

This operator has equal deficiency indices

$$(d_+, d_-) = (2|\mathcal{I}_d| + |\mathcal{I}_t|, 2|\mathcal{I}_d| + |\mathcal{I}_t|)$$

and hence there are self–adjoint extensions. Its adjoint $S = (S^0)^*$ in the Hilbert space $\mathcal{H}$ is formally the same operator but with domain $\mathrm{Dom}(S) = \mathcal{D}_d \oplus \mathcal{W}_t$. Self–adjoint extensions $\widetilde{S}$ of S^0 lie between the minimal and the maximal operator

$$S^0 \subset \widetilde{S} \subset S.$$

Consequently all self–adjoint extensions can be parametrized in terms of boundary conditions. One defines the appropriately modified vectors of boundary values

$$\bar{u} := \begin{bmatrix} \{u_{di}(a_{di})\}_{1\leq i\leq D} \\ \{u_{di}(0)\}_{1\leq i\leq D} \\ 2^{-\frac{1}{2}}\{u_{tj}(a_{tj}) + u_{tj}(0)\}_{1\leq j\leq T} \end{bmatrix}, \ \bar{\bar{u}} := \begin{bmatrix} \{u_{di}'(a_{di})\}_{1\leq i\leq D} \\ \{-u_{di}'(0)\}_{1\leq i\leq D} \\ i2^{-\frac{1}{2}}\{-u_{tj}(a_{tj}) + u_{tj}(0)\}_{1\leq j\leq T} \end{bmatrix},$$

where $\bar{u}, \bar{\bar{u}} \in \underline{\mathcal{K}}$. To measure how far the maximal operator S is from being self–adjoint consider

$$\langle Su, v\rangle - \langle u, Sv\rangle = \left\langle \begin{bmatrix} \bar{u} \\ \bar{\bar{u}} \end{bmatrix}, \begin{bmatrix} 0 & -\mathbb{1}_{\underline{\mathcal{K}}} \\ \mathbb{1}_{\underline{\mathcal{K}}} & 0 \end{bmatrix} \begin{bmatrix} \bar{v} \\ \bar{\bar{v}} \end{bmatrix} \right\rangle_{\underline{\mathcal{K}}^2},$$

where $u, v \in \mathcal{D}_d \oplus \mathcal{W}_t$. The right hand side defines the standard Hermitian symplectic form in the space of boundary values $\underline{\mathcal{K}}^2$. Without going into detail one can state that there is a one–to–one correspondence between the maximal isotropic subspaces with respect to this Hermitian symplectic form and the self–adjoint extensions of S^0, see for example [47]. A unique parametrization of such a maximal isotropic subspace in $\underline{\mathcal{K}}^2$ can be given in terms of a projection P in $\underline{\mathcal{K}}$ and a Hermitian operator L acting in the subspace $\operatorname{Ran} P^{\perp}$, compare [72]. Therefore an arbitrary self–adjoint realization $\widetilde{S}$ of S^0 is a restriction of S, which satisfies certain boundary conditions of the form

$$P\bar{u} = 0 \quad \text{and} \quad L\bar{u} + P^{\perp}\bar{\bar{u}} = 0.$$

Thus one sets $\widetilde{S} = S_{P,L}$.

The spectrum of the self–adjoint operator $S_{P,L}$ is purely discrete and there are sequences of eigenvalues going to $+\infty$ as well as to $-\infty$. A more detailed analysis of the spectrum can be performed on the lines of Section 3.2. Such a self–adjoint operator can be interpreted as Hamiltonian consisting of a standard Laplacian and the less usual moment–type observable. Moment operators on graphs have been recently studied in the article [35].

By Stone's theorem, for a self–adjoint operator $S_{P,L}$ the Cauchy problem

$$\begin{cases} \left(i\dfrac{\partial}{\partial t} - S_{P,L}\right) u(x,t) = 0, \\ \\ u(\cdot, 0) = u_0, \quad \text{for } t \in \mathbb{R} \end{cases}$$

is governed by the unitary group given by $U(t) = e^{-itS_{P,L}}$, which delivers the time–dependent solution $u(\cdot, t) = U(t)u_0$.

3.4.2. Dirac and Schrödinger equation. Another example for mixed dynamics is a network where the dynamics is given on some edges by the one–dimensional Schrödinger equation and on the rest of the edges by the one–dimensional Dirac equation. As already remarked the Schrödinger equation on graphs is studied intensely. Self–adjoint Dirac operators on graphs are studied for example in [20, 80]. The coupling of both is a new feature.

In mesoscopic scales the behaviour of an electron can be described by the Schrödinger equation, see for example [27] and the references therein. However in certain, more specific mesoscopic models like the one of carbon nanotubes and more general carbon latices the behaviour of an electron can be described formally by the Dirac equation, see for example [31, 77, 99] and the references given therein. For further information and references about the scattering theory of Dirac operators and related models in mesoscopic physics, see also [50] and the references therein.

In this context one can think – hypothetically – of a system which is described partially by the Dirac equation and partially by the Schrödinger equation. This could arise by coupling a "usual" mesoscopic system with carbon nanotubes. In the reduced situation of graphs one can consider a network, which is modeled by a metric graph $\mathcal{G}$ consisting of two parts. On $\mathcal{G}_D$ the dynamic is described by the Dirac equation and on the part $\mathcal{G}_S$ the time–evolution is governed by the Schrödinger equation. As in the previous models, it is assumed that interactions of both are taking place only at the vertices.

For simplicity consider a star graph $\mathcal{G} = (V, \mathcal{E}, \partial)$ with division

$$\mathcal{E} = \mathcal{E}_S \dot{\cup} \mathcal{E}_D,$$

where on $\mathcal{E}_S$ the Schrödinger equation is considered and on $\mathcal{E}_D$ the Dirac equation. To formalize this consider the Hilbert spaces

$$\widetilde{\mathcal{H}} = \mathcal{H}(\mathcal{E}_S) \oplus \mathcal{H}^2(\mathcal{E}_D),$$

where $\mathcal{H}^2(\mathcal{E}_D)$ has been defined in (7). Any element $u \in \widetilde{\mathcal{H}}$ can be written with respect to this decomposition as

$$u = \begin{bmatrix} u_S \\ u_D \end{bmatrix}, \quad \text{where } u_S \in \mathcal{H}(\mathcal{E}_S) \text{ and } u_D \in \mathcal{H}(\mathcal{E}_D).$$

The minimal operator H^0 is defined by

$$H^0 := \begin{bmatrix} -\Delta & 0 \\ 0 & D \end{bmatrix}$$

with

$$\mathrm{Dom}(H^0) = \mathcal{D}^0(\mathcal{E}_S) \oplus \mathcal{W}_0^2(\mathcal{E}_D),$$

where D denotes the Dirac operator defined in (10). Observing that the adjoint $H = (H^0)^*$ is formally the same operator, but defined on the larger space

$$\mathrm{Dom}(H) = \mathcal{D}(\mathcal{E}_S) \oplus \mathcal{W}^2(\mathcal{E}_D)$$

one can find all self–adjoint extensions of H^0 using the same methods from extension theory that were used in the previous example. Note that H^0 has equal deficiency indices

$$(d_+, d_-) = (|\mathcal{E}_S| + |\mathcal{E}_D|, |\mathcal{E}_S| + |\mathcal{E}_D|).$$

One defines the appropriately modified vectors of boundary values

$$\underline{u} := \begin{bmatrix} \underline{u}_S \\ \underline{u}_D \end{bmatrix} \quad \text{and} \quad \underline{u}' := \begin{bmatrix} \underline{u}'_S \\ \underline{u}'_D \end{bmatrix}$$

with

$$\underline{u}_S = \{u_e(0)\}_{e \in \mathcal{E}_S}, \qquad \underline{u}'_S = \{u'_e(0)\}_{e \in \mathcal{E}_S}$$

and

$$\underline{u}_D = \{u_e^1(0)\}_{e \in \mathcal{E}_D}, \qquad \underline{u}'_D = \{u_e^2(0)\}_{e \in \mathcal{E}_D}.$$

An appropriate space of boundary values is

$$\widetilde{\mathcal{K}} \equiv \widetilde{\mathcal{K}}(\mathcal{E}_S, \mathcal{E}_D) = \mathcal{K}(\mathcal{E}_S) \oplus \mathcal{K}(\mathcal{E}_D),$$

where $\mathcal{K}(\mathcal{E}_S) \cong \mathbb{C}^{|\mathcal{E}_S|}$ and $\mathcal{K}(\mathcal{E}_D) \cong \mathbb{C}^{|\mathcal{E}_D|}$. Clearly $\underline{u}, \underline{u}' \in \widetilde{\mathcal{K}}$. Again the well known standard Hermitian symplectic form on the space of boundary values appears when considering the difference

$$\langle Hu, v \rangle - \langle u, Hv \rangle = \left\langle \begin{bmatrix} \underline{u} \\ \underline{u}' \end{bmatrix}, \begin{bmatrix} 0 & -\mathbb{1}_{\widetilde{\mathcal{K}}} \\ \mathbb{1}_{\widetilde{\mathcal{K}}} & 0 \end{bmatrix} \begin{bmatrix} \underline{v} \\ \underline{v}' \end{bmatrix} \right\rangle_{\widetilde{\mathcal{K}}^2},$$

where $u, v \in \mathrm{Dom}(H)$. A unique parametrization of a maximal isotropic subspace is given in terms of a projection P in $\widetilde{\mathcal{K}}$ and a Hermitian operator L acting in the space $\mathrm{Ran}\, P^\perp$. Therefore any self–adjoint realization $\widetilde{H}$ of H^0 is a restriction of H onto a domain of the type

$$\mathrm{Dom}(H_{P,L}) = \{u \in \mathcal{D}(\mathcal{E}_S) \oplus \mathcal{W}^2(\mathcal{E}_D) \mid P\underline{u} = 0 \text{ and } L\underline{u} + P^\perp \underline{u}' = 0\},$$

and one sets $\widetilde{H} = H_{P,L}$. These are all self–adjoint boundary conditions, but the question which of these are in some sense *natural* remains unanswered like in the above cases of mixed dynamics. The time–dependent solutions of the Cauchy problem

$$\begin{cases} \left(i\dfrac{\partial}{\partial t} - H_{P,L}\right) u(x,t) = 0, \\ \\ u(\cdot,0) = u_0, \quad \text{for } t \in \mathbb{R} \end{cases}$$

is $u(\cdot,t) = U(t)u_0$, where $U(t) = e^{-itH_{P,L}}$.

3.4.3. Time–reversed Schrödinger equation. Consider a star graph $\mathcal{G}$ with $\mathcal{E} = \mathcal{E}_+ \cup \mathcal{E}_-$. In the subsequent chapter the self–adjoint operator $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ in $L^2(\mathbb{R})$ is interpreted as a system of mixed dynamic of the type

$$\tau = \begin{bmatrix} -\Delta & 0 \\ 0 & +\Delta \end{bmatrix}$$

given with respect to the decomposition $\mathcal{E} = \mathcal{E}_+ \cup \mathcal{E}_-$. Generalisations to finite metric graphs are introduced. An answer to the question of natural boundary conditions is proposed using indefinite quadratic forms. Operators of this type appear in applications to metamaterials and in solid-state physics. A self–adjoint realization T of τ generates a unitary group given by $U(t) = e^{-itT}$, which provides solutions for the initial value problem

$$\begin{cases} \left(i\dfrac{\partial}{\partial t} - T\right) u(x,t) = 0, \\ \\ u(\cdot,0) = u_0, \quad \text{for } t \in \mathbb{R}. \end{cases}$$

Compared to the time–dependent behaviour of groups generated by (positive) self–adjoint Laplacians $-\Delta$, the group generated by T describes the time–reversed behaviour on the negative edges $\mathcal{E}_-$ and the forward–directed behaviour on the positive edges $\mathcal{E}_+$.

CHAPTER 4

Indefinite second order differential operators

Differential expressions of the form

$$-\operatorname{div} A(\cdot) \operatorname{grad} \quad \text{with} \quad A(x) = \begin{cases} +1, & x \in \Omega_+, \\ -1, & x \in \Omega_-, \end{cases} \tag{52}$$

for domains $\Omega = \Omega_+ \cup \Omega_- \subset \mathbb{R}^d$ appear in different contexts. The Poisson problem related to this operator is of physical relevance. It appears in the mathematical description of light propagation through regions with thresholds of materials with negative refraction index and positive refraction index, see [22] and the references therein. The quasi–static limit of the Maxwell equation yields the mentioned Poisson problem. Another field of application is solid-state physics. In the effective mass approximation the effective mass tensor can have changing sign as well. This yields indefinite differential operators, which involve expressions of the form (52) and in this context the Schrödinger equation is considered, see for example [3] and the references therein.

An approach that has turned out to be very fruitful for the study of differential equations which involve strictly positive coefficient matrices $A(\cdot)$, is to consider self–adjoint operators associated with differential expressions and their spectral resolution. The question is, if it is possible to study equations involving expressions of the form (52) in terms of spectral theory also for indefinite coefficients $A(\cdot)$. Unbounded operators with sign changing coefficients in the highest order term are not well studied. To make a starting point a new model problem is proposed: Laplace operators on finite metric graphs with changing sign. The aim of this chapter is to present generalizations of the model operator

$$-\frac{d}{dx} \operatorname{sign}(x) \frac{d}{dx} \quad \text{with} \quad \operatorname{sign}(x) = \begin{cases} +1, & x \geq 0, \\ -1, & x < 0 \end{cases} \tag{53}$$

to finite metric graphs. The self–adjoint realisations of these are completely characterized and the spectral and scattering theory is developed.

A similar procedure has been performed already very successfully for the sign definite one dimensional Laplacian. The generalisation to metric graphs has become famous under the name "quantum graphs". For further references on this topic see for example [14] and the references cited therein. Observe that the model problem (53) is part of a range of problems related to the ordinary differential expressions

$$\begin{aligned} -\frac{d^2}{dx^2}, \qquad & -\frac{d}{dx} \operatorname{sign}(x) \frac{d}{dx}, \\ -\operatorname{sign}(x) \frac{d^2}{dx^2} \quad \text{and} \quad & -\operatorname{sign}(x) \frac{d}{dx} \operatorname{sign}(x) \frac{d}{dx}. \end{aligned}$$

Each is exemplary for certain difficulties and methods used. Usually the operators in the first line are considered in Hilbert spaces, whereas the operators in the second line are considered in Krein spaces, see for example [25, 97]. The operator $-\operatorname{sign}(x)\frac{d^2}{dx^2}$ has applications in the effective mass approximation too, compare [100].

The initial problem given in (53) can be tackled using an extension theory approach, which allows straight forward generalizations from intervals to finite metric graphs. The first step is to rewrite the operator. Instead of considering the operator given in (53) in the Hilbert space $L^2(\mathbb{R}, dx)$, one considers in the equivalent space

$$L^2([0,\infty), dx_1) \oplus L^2([0,\infty), dx_2) \quad (\cong L^2(\mathbb{R}, dx))$$

the formal differential operator

$$\tau u = (+u_1'', -u_2'').$$

This gives rise to the definition of a closed symmetric (minimal) operator with equal deficiency indices $(2,2)$. Hence there exist self-adjoint extensions. Adapting the methods known from the theory of Laplace operators on finite metric graphs one arrives at parametrizations of all self-adjoint extensions. Then one can develop the spectral and scattering theory of these operators on the lines of the theory of Laplacians on finite metric graphs, see for example [62,63] and similar to the theory of point interactions, see for example [2] and the references therein.

Some aspects of this problem are included in the general setting of Sturm-Liouville theory, but they have been considered to have no practical relevance, as remarked in [91, Section 17.E]. The motivation to consider the problem is caused mainly by the fast development in the field of so called metamaterials – materials with negative optical refraction index. This has been initiated by V. G. Veselago, see [90], who was the first to consider – hypothetically – the effect of a negative refraction index. He had predicted that this feature would yield new effects including for example backward waves, an inverse law of refraction and an inverse Doppler effect. Today metamaterials can be constructed as artificial materials, whose optical properties are made useful for applications. An overview of recent developments is given in the article [86].

The intention of this chapter is to provide a model problem for indefinite differential operators, generated by expressions of the form (52). On finite metric graphs this gives a model, which on the one hand is still explicitly solvable, but on the other hand it allows to describe more complicated geometries than only intervals. The aim is to develop a better understanding of the spectral properties of sign–indefinite differential operators.

The chapter is organized as follows: the first section is devoted to the characterization of self-adjoint boundary conditions for the indefinite model–operator. In short the corresponding question for self–adjointness in Krein spaces is discussed as well. Section 4.2 puts the question of self-adjoint extensions into the context of indefinite quadratic forms and adapts the approach which is going to be presented in [56] to the situation considered here. In the subsequent section the operators discussed are put into the general context of extension theory. Section 4.4 gives explicit formulae for eigenvalues, resonances and resolvents. In Section 4.5 the scattering properties of the system are discussed. The wave operators as well as the scattering matrix are computed and in certain cases the scattering matrix can be computed in terms of a generalized star product.

The content of this chapter has developed in parallel to the work on the article [56], which is in preparation. The content of [56] is partially included in Part 2 of this thesis. The indefinite operators on graphs considered here served for me as an illustration and a source of examples for indefinite operators on bounded domains and intervals. Parts of this chapter are also available as preprint, see [52].

4.1. Self–adjoint realizations

Consider the finite graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ endowed with the metric structure $\underline{a}$. One distinguishes two types of edges

$$\mathcal{E} = \mathcal{E}_+ \dot\cup \mathcal{E}_- \quad \text{and} \quad \mathcal{I} = \mathcal{I}_+ \dot\cup \mathcal{I}_-,$$

where $\mathcal{E}_+$ ($\mathcal{E}_-$) and $\mathcal{I}_+$ ($\mathcal{I}_-$) are called the *positive (negative) external edges* and *positive (negative) internal edges*, respectively. The set $\mathcal{E}_+ \cup \mathcal{I}_+$ ($\mathcal{E}_- \cup \mathcal{I}_-$) denotes the *positive (negative) edges*. This partition defines two sub–graphs

$$\mathcal{G}_-, \mathcal{G}_+ \subset \mathcal{G}, \quad \text{where} \quad \mathcal{G}_\pm = (V_\pm, \mathcal{I}_\pm, \mathcal{E}_\pm, \partial\,|_{(\mathcal{E}_\pm \cup \mathcal{I}_\pm)})$$

with $V_\pm = \partial(\mathcal{E}_\pm \cup \mathcal{I}_\pm)$. Let be $\underline{a}_\pm = \{a_i\}_{i \in \mathcal{I}_\pm}$, then $(\mathcal{G}_\pm, \underline{a}_\pm)$ are metric graphs. For brevity set

$$m = 2|\mathcal{I}_-| + |\mathcal{E}_-| \quad \text{and} \quad n = 2|\mathcal{I}_+| + |\mathcal{E}_+|.$$

4.1.1. The minimal and the maximal operator. Given a finite metric graph $(\mathcal{G}, \underline{a})$ one considers the Hilbert space

$$\mathcal{H} \equiv \mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}_\mathcal{E} \oplus \mathcal{H}_\mathcal{I}, \quad \mathcal{H}_\mathcal{E} = \bigoplus\nolimits_{e \in \mathcal{E}} \mathcal{H}_e, \quad \mathcal{H}_\mathcal{I} = \bigoplus_{i \in \mathcal{I}} \mathcal{H}_i,$$

defined in (4). Again one has a decomposition into two subspaces

$$\mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}(\mathcal{E}_+, \mathcal{I}_+, \underline{a}_+) \oplus \mathcal{H}(\mathcal{E}_-, \mathcal{I}_-, \underline{a}_-),$$

where one sets for brevity $\mathcal{H}_+ = \mathcal{H}(\mathcal{E}_+, \mathcal{I}_+, \underline{a}_+)$ and $\mathcal{H}_- = \mathcal{H}(\mathcal{E}_-, \mathcal{I}_-, \underline{a}_-)$. One considers the formal differential operator τ defined by

$$(\tau\psi)_j(x) = \begin{cases} -\frac{d^2}{dx}\psi_j(x), & j \in \mathcal{E}_+ \cup \mathcal{I}_+,\ x \in I_j, \\ +\frac{d^2}{dx}\psi_j(x), & j \in \mathcal{E}_- \cup \mathcal{I}_-,\ x \in I_j. \end{cases}$$

That is τ acts as $-\Delta$ on $(\mathcal{G}_+, \underline{a}_+)$ and as $+\Delta$ on $(\mathcal{G}_-, \underline{a}_-)$. To emphasise the importance of domains and to make the choice of the domains transparent, the notation to write a differential operator as 2-tuple, consisting of a differential expression and a domain is used in this chapter. The operator

$$T^{\min} = (\tau, \mathcal{D}^0)$$

is closed, densely defined and symmetric. Its adjoint in the Hilbert space $\mathcal{H}$ is the operator $T^{\max} = \left(T^{\min}\right)^*$,

$$T^{\max} = (\tau, \mathcal{D}).$$

Since the operator $T^{\min}$ has equal deficiency indices

$$(d_+, d_-) = (d, d), \quad \text{where } d = n + m,$$

there are self-adjoint realizations $T = T^*$ of τ with

$$T^{\min} \subset T \subset T^{\max}.$$

On the lines of (12) one introduces the auxiliary Hilbert spaces

$$\mathcal{K}_\pm \equiv \mathcal{K}(\mathcal{E}_\pm, \mathcal{I}_\pm) = \mathcal{K}_{\mathcal{E}_\pm} \oplus \mathcal{K}_{\mathcal{I}_\pm}^- \oplus \mathcal{K}_{\mathcal{I}_\pm}^+$$

with $\mathcal{K}_{\mathcal{E}_\pm} \cong \mathbb{C}^{|\mathcal{E}_\pm|}$ and $\mathcal{K}_{\mathcal{I}_\pm}^{(\pm)} \cong \mathbb{C}^{|\mathcal{I}_\pm|}$. Finally one defines

$$\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_- \quad \text{and} \quad \mathcal{K}^2 = \mathcal{K} \oplus \mathcal{K}.$$

Let be given an operator acting in the space $\mathcal{K}$ or $\mathcal{K}^2$, then the distinction between $\mathcal{K}_+$ and $\mathcal{K}_-$ induces a block structure on this operator. This is an instrument frequently used to perform explicit calculations.

For $\psi \in \mathcal{D}$ one defines the vectors of boundary values

$$\underline{\psi}_+ = \begin{bmatrix} \{\psi_j(0)\}_{j\in\mathcal{E}_+} \\ \{\psi_j(0)\}_{j\in\mathcal{I}_+} \\ \{\psi_j(a_j)\}_{j\in\mathcal{I}_+} \end{bmatrix}, \quad \underline{\psi}_- = \begin{bmatrix} \{\psi_j(0)\}_{j\in\mathcal{E}_-} \\ \{\psi_j(0)\}_{j\in\mathcal{I}_-} \\ \{\psi_j(a_j)\}_{j\in\mathcal{I}_-} \end{bmatrix}, \quad \underline{\psi} = \begin{bmatrix} \underline{\psi}_+ \\ \underline{\psi}_- \end{bmatrix},$$

$$\underline{\psi}'_+ = \begin{bmatrix} \{\psi'_j(0)\}_{j\in\mathcal{E}_+} \\ \{\psi'_j(0)\}_{j\in\mathcal{I}_+} \\ \{-\psi'_j(a_j)\}_{j\in\mathcal{I}_+} \end{bmatrix}, \quad \underline{\psi}'_- = \begin{bmatrix} \{\psi'_j(0)\}_{j\in\mathcal{E}_-} \\ \{\psi'_j(0)\}_{j\in\mathcal{I}_-} \\ \{-\psi'_j(a_j)\}_{j\in\mathcal{I}_-} \end{bmatrix}, \quad \underline{\psi}' = \begin{bmatrix} \underline{\psi}'_+ \\ \underline{\psi}'_- \end{bmatrix}.$$

The vector $[\psi] = \underline{\psi} \oplus \underline{\psi}'$ is an element of $\mathcal{K}^2 = \mathcal{K} \oplus \mathcal{K}$.

4.1.2. Hermitian symplectic forms. To measure how far the maximal operator $T^{\max}$ is away from being self-adjoint one evaluates the form $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$ defined by

$$\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}(\psi,\varphi) := \langle T^{\max}\psi, \varphi\rangle - \langle \psi, T^{\max}\varphi\rangle, \quad \text{for } \psi,\varphi \in \mathcal{D},$$

compare for example [47, Section 3]. This form can be represented by a matrix on the finite dimensional space $\mathcal{K}^2$. This gives

$$\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}(\psi,\varphi) = \langle [\psi], \mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)}[\varphi]\rangle_{\mathcal{K}^2},$$

where the matrix

$$\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)} = \begin{bmatrix} 0 & 0 & -\mathbb{1}_n & 0 \\ 0 & 0 & 0 & \mathbb{1}_m \\ \mathbb{1}_n & 0 & 0 & 0 \\ 0 & -\mathbb{1}_m & 0 & 0 \end{bmatrix},$$

is written with respect to the decomposition of $\mathcal{K}^2 = \mathcal{K}_+ \oplus \mathcal{K}_- \oplus \mathcal{K}_+ \oplus \mathcal{K}_-$; $\mathbb{1}_n$ denotes the identity operator in the n-dimensional space $\mathcal{K}_+$ and $\mathbb{1}_m$ the identity in the m-dimensional space $\mathcal{K}_-$, respectively. By an abuse of notation one denotes by $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$ also the sesquilinear form defined by $\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)}$ on $\mathcal{K}^2$. Notice that

$$\mathfrak{J}^*_{(\mathcal{G}_+,\mathcal{G}_-)} = -\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)} \quad \text{and} \quad \mathfrak{J}^2_{(\mathcal{G}_+,\mathcal{G}_-)} = -\mathbb{1}_{\mathcal{K}^2}$$

holds and therefore $\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)}$ is a Hermitian symplectic matrix in $\mathcal{K}^2$. The relation to the standard Hermitian symplectic matrix

$$\mathfrak{J}_{\mathcal{G}} = \begin{bmatrix} 0 & 0 & -\mathbb{1}_n & 0 \\ 0 & 0 & 0 & -\mathbb{1}_m \\ \mathbb{1}_n & 0 & 0 & 0 \\ 0 & \mathbb{1}_m & 0 & 0 \end{bmatrix}$$

is summarized in the following

LEMMA 4.1. *The following similarity relations hold*

$$\mathfrak{J}_{\mathcal{G}} = \Pi_{n,m}\,\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)}\,\Pi_{n,m} \quad \textit{and} \quad \mathfrak{J}_{\mathcal{G}} = H_{n,m}\,\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)}\,H_{n,m},$$

where the matrices involved are written with respect to the decomposition of $\mathcal{K}^2 = \mathcal{K}_+ \oplus \mathcal{K}_- \oplus \mathcal{K}_+ \oplus \mathcal{K}_-$ *as*

$$\Pi_{n,m} = \begin{bmatrix} \mathbb{1}_n & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{1}_m \\ 0 & 0 & \mathbb{1}_n & 0 \\ 0 & \mathbb{1}_m & 0 & 0 \end{bmatrix} \quad \textit{and} \quad H_{n,m} := \begin{bmatrix} \mathbb{1}_n & 0 & 0 & 0 \\ 0 & \mathbb{1}_m & 0 & 0 \\ 0 & 0 & \mathbb{1}_n & 0 \\ 0 & 0 & 0 & -\mathbb{1}_m \end{bmatrix}.$$

A space $\mathcal{M} \subset \mathcal{K}^2$ is called *maximal isotropic with respect to* $\mathfrak{j}_{\mathcal{G}_+,\mathcal{G}_-}$ if

$$\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}(\xi_1,\xi_2) = \left\langle \xi_1, \mathfrak{J}_{\mathcal{G}_+,\mathcal{G}_-}\,\xi_2 \right\rangle = 0 \quad \text{for all} \quad \xi_1,\xi_2 \in \mathcal{M}$$

and there are no proper subspaces $\mathcal{M} \subsetneq \mathcal{M}'$ having this property, compare [47, Definitions 7 and 8, and the following]. From Lemma 4.1 one deduces a one–to–one correspondence between subspaces in $\mathcal{K}^2$ which are maximal isotropic with respect to the standard Hermitian symplectic form, which is well studied, and subspaces in $\mathcal{K}^2$ that are maximal isotropic with respect to the Hermitian symplectic form $\mathfrak{j}_{\mathcal{G}_+,\mathcal{G}_-}$ occurring here.

Any subspace $\mathcal{M} \subset \mathcal{K}^2$ with $\dim \mathcal{M} \geq d$ can be parametrized as follows. Let A and B be linear maps in $\mathcal{K}$. By $(A,\,B)$ one denotes the linear map from $\mathcal{K}^2 = \mathcal{K} \oplus \mathcal{K}$ to $\mathcal{K}$ defined by $(A,\,B)(\eta_1 \oplus \eta_2) = A\eta_1 + B\eta_2$, where $\eta_1, \eta_2 \in \mathcal{K}$. One sets

$$\mathcal{M} = \mathcal{M}(A,B), \quad \text{where} \quad \mathcal{M}(A,B) = \operatorname{Ker}(A,\,B).$$

The more general relation between self–adjoint extensions and Hermitian symplectic geometry is discussed in the article [47].

THEOREM 4.2. *All self–adjoint extensions of $T^{\min}$ are uniquely determined by subspaces $\mathcal{M} \subset \mathcal{K}^2$, which are maximal isotropic with respect to the Hermitian symplectic form $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$. All such maximal isotropic subspaces are given by $\mathcal{M} = \mathcal{M}(A,B)$, where A and B are linear maps in $\mathcal{K}$, which satisfy the two conditions*

(1) *Rank $(A,\,B) = n+m$, that is the rank maximal and*
(2) *$BJ_{n,m}A^* = AJ_{n,m}B^*$, where*

$$J_{n,m} := \begin{bmatrix} \mathbb{1}_n & 0 \\ 0 & -\mathbb{1}_m \end{bmatrix}$$

defines a map in $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$.

Any self–adjoint extension of $T^{\min}$ is given by

$$T(A,B) = (\tau, \operatorname{Dom}(T(A,B)))$$

with

$$\operatorname{Dom}(T(A,B)) = \left\{ \psi \in \mathcal{D} \mid A\underline{\psi} + B\underline{\psi}' = 0 \right\},$$

where A, B satisfy both conditions (1) and (2).

REMARK 4.3.

(1) *The condition $A\underline{\psi} + B\underline{\psi}' = 0$ is equivalent to $[\psi] \in \mathcal{M}(A,B)$.*
(2) *The operator $-\overline{T(A,B)}$ is the operator with positive and negative edges interchanged, but the coupling is implemented by the same boundary conditions at the vertices.*

(3) *For $\mathcal{G}_{\mp} = \emptyset$ the operator $T(A,B)$ is the self-adjoint operator plus or minus Laplace $\mp\Delta(A,B)$ on $\mathcal{G}_{\pm}$.*

(4) *Observe that the second condition can be re–formulated in terms of relations in finite dimensional Krein spaces. Consider the space $\mathcal{K}$ equipped with the indefinite inner product $[\cdot,\cdot] = \langle \cdot, J_{n,m}\cdot\rangle_{\mathcal{K}}$. Then $BJ_{n,m}A^* = BA^{[*]}$, where $\cdot^{[*]}$ denotes the Krein space adjoint.*

REMARK 4.4 (An application to Laplace operators on finite metric graphs). *Let $-\Delta(A,B)$ be a self–adjoint Laplacian on a star graph $\mathcal{G}$. To decide whether the boundary conditions couple functions defined on two sub–graphs $\mathcal{G}_+$, $\mathcal{G}_-$ or not, one has to compute the local scattering matrix*

$$\mathfrak{S}(k;A,B) = -\left(A + ikB\right)^{-1}\left(A - ikB\right), \quad k > 0,$$

defined for example in [60]. This can be a costly task, because it involves the inversion of a possibly large matrix. The space $\mathcal{M}(A,B)$ is maximal isotropic with respect to both $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$ and the standard Hermitian symplectic form if and only if it defines the two self–adjoint operators $-\Delta(A,B)$ and $T(A,B)$ simultaneously. This is possible if and only if the boundary conditions defined by A,B decouple positive from negative edges. Consequently the two sub–graphs $\mathcal{G}_+$ and $\mathcal{G}_-$ are not matched together by these boundary conditions if and only if both $BJ_{n,m}A^*$ and BA^* are Hermitian. This condition is much easier to verify than to compute the local scattering matrix.

PROOF OF THEOREM 4.2. Let T be an extension of $T^{\min}$ with

$$T^{\min} \subset T \subset T^{\max}.$$

For symmetric T the form $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$ must vanish identically on $\mathrm{Dom}(T)$. From the classical theory for extensions of symmetric operators with finite deficiency indices it follows that the self–adjoint extensions are given by $d = n+m$ dimensional subspaces of the space of boundary values, see for example [92, Theorem 10.10], [18, Theorem 4.9.2] or [47]. Hence all subspaces $\mathcal{M}$ of $\mathcal{K}^2$, which are maximal isotropic with respect to the Hermitian symplectic form $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$ define self-adjoint extensions of the operator $T^{\min}$. On the other hand, given a self-adjoint extension, it defines a d–dimensional subspace in the space of boundary values on which the form $\mathfrak{j}_{(\mathcal{G}_+,\mathcal{G}_-)}$ is constantly zero. Hence it is maximal isotropic with respect to this form.

To prove the parametrization, let now $\mathcal{M}$ be a maximal isotropic subspace of $\mathcal{K}^2$ with respect to the Hermitian symplectic form defined by $\mathfrak{J}_{(\mathcal{G}_+,\mathcal{G}_-)}$. Then by Lemma 4.1 the space $H_{n,m}\mathcal{M}$ is a maximal isotropic subspace of $\mathcal{K}^2$ with respect to the standard Hermitian symplectic form defined by $\mathfrak{J}_{\mathcal{G}}$. The space $H_{n,m}\mathcal{M}$ can be parametrized by matrices A_0, B_0, see for example [60], which satisfy the two conditions

(1) $\mathrm{Rank}(A_0,\, B_0) = n+m$ and
(2) $B_0A_0^* = B_0A_0^*$.

Hence the original space $\mathcal{M}$ can be represented as

$$\mathcal{M} = H_{n,m}\,\mathrm{Ker}\,(A_0,\, B_0) = \mathrm{Ker}\left(A_0,\, B_0\begin{bmatrix}\mathbb{1}_n & 0\\ 0 & -\mathbb{1}_m\end{bmatrix}\right),$$

where the matrices

$$A = A_0 \quad \text{and} \quad B = B_0\begin{bmatrix}\mathbb{1}_n & 0\\ 0 & -\mathbb{1}_m\end{bmatrix}$$

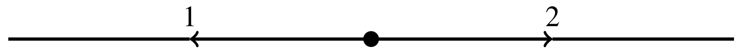


FIGURE 3. The graph in Example 4.7.

satisfy the two conditions formulated in Theorem 4.2 and $\mathcal{M} = \mathcal{M}(A, B)$. □

The parametrization by matrices A and B in Theorem 4.2 is not unique, since two operators $T(A', B')$ and $T(A, B)$ are equal if and only if the corresponding subspaces $\mathcal{M}(A', B')$ and $\mathcal{M}(A, B)$ agree. Using the result [72, Theorem 6] on self-adjoint Laplacians on finite metric graphs, one obtains a unique parametrization.

COROLLARY 4.5. *Let $\mathcal{M}(A, B) \subset \mathcal{K}^2$ be maximal isotropic with respect to the Hermitian symplectic form $\jmath_{(\mathcal{G}_+,\mathcal{G}_-)}$. Then there exists a unique orthogonal projection P and a unique Hermitian operator L with $P^\perp L P^\perp = L$, where $P^\perp = \mathbb{1} - P$, such that with*

$$A' = L + P \quad \textit{and} \quad B' = P^\perp \begin{bmatrix} \mathbb{1}_n & 0 \\ 0 & -\mathbb{1}_m \end{bmatrix}$$

one has $\mathcal{M}(A, B) = \mathcal{M}(A', B')$. Here, P is the orthogonal projector to $\operatorname{Ker} B J_{n,m} \subset \mathcal{K}$.

REMARK 4.6. *The proof of Theorem 4.2 shows that if one has a self–adjoint Laplace operator $-\Delta(A_0, B_0)$ parametrized by matrices A_0 and B_0, then $T(A, B)$ is self–adjoint with*

$$A = A_0 \quad \textit{and} \quad B = B_0 J_{n,m}.$$

In particular, there is a unique parametrization in terms of unitary operators in $\mathcal{K}$. For Laplace operators it is known that for self–adjoint boundary conditions defined by operators A_0 and B_0 in $\mathcal{K}$ there exists a unique unitary map U in $\mathcal{K}$ such that equivalent boundary conditions are defined by

$$A_0' = -\frac{1}{2}(U - \mathbb{1}) \quad \textit{and} \quad B_0' = \frac{1}{2i}(U + \mathbb{1}),$$

compare for example [47, Section 3]. Hence for $T(A, B)$ self–adjoint one can give an equivalent parametrization in terms of the same unitary matrix U with

$$A' = -\frac{1}{2}(U - \mathbb{1}) \quad \textit{and} \quad B' = \frac{1}{2i}(U + \mathbb{1}) J_{n,m}.$$

EXAMPLE 4.7. *Let $\mathcal{G}$ be the star graph consisting of two external edges, $\mathcal{E}_+ = \{1\}$ and $\mathcal{E}_- = \{2\}$, glued together at one single vertex $\partial(1) = \partial(2)$. Consider*

$$A = \begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix} \quad \textit{and} \quad B = \begin{bmatrix} 0 & 0 \\ -1 & 1 \end{bmatrix}. \tag{54}$$

Since A, B satisfy the two conditions formulated in Theorem 4.2 the space $\mathcal{M}(A, B)$ is maximal isotropic with respect to the form $\jmath_{(\mathcal{G}_+,\mathcal{G}_-)}$ and hence the operator $T(A, B)$ is self–adjoint. One can identify the metric graph $\mathcal{G}$ with the real line, and under this identification the operator $T(A, B)$ corresponds to the operator

$$-\tfrac{d}{dx} \operatorname{sign}(x) \tfrac{d}{dx}$$

defined in $L^2(\mathbb{R}; \mathbb{C})$ on its natural domain.

4.1.3. Self-adjointness in Krein spaces. One can consider the same graph $\mathcal{G}$ given in Example 4.7, but one imposes boundary conditions which are defined by

$$A = \begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}.$$

These define the non–self–adjoint operator $T(A,B)$ and the self–adjoint operator $-\Delta(A,B)$. The operator $T(A,B)$ corresponds, again by identifying the metric graph $\mathcal{G}$ with the real line, to the non–self–adjoint operator $-\operatorname{sign}(x)\frac{d^2}{dx^2}$ with domain $H^2(\mathbb{R};\mathbb{C}) \subset L^2(\mathbb{R};\mathbb{C})$. A generalization of $-\operatorname{sign}(x)\frac{d^2}{dx^2}$ from intervals to finite metric graphs can be done on the same lines as for $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$. Define the Krein space

$$\mathfrak{K} = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} L^2(I_j), \quad \text{with indefinite inner product} \quad [\cdot,\cdot]_{\mathfrak{K}} = \langle \cdot, J_{n,m}\cdot\rangle_{\mathcal{H}},$$

where with a slight abuse of notation one sets

$$(J_{n,m}\psi)_j = \begin{cases} +\psi_j, & j \in \mathcal{E}_+ \cup \mathcal{I}_+, \\ -\psi_j, & j \in \mathcal{E}_- \cup \mathcal{I}_-. \end{cases}$$

The multiplication with $J_{n,m}$ is the fundamental symmetry of the Krein space $\mathfrak{K}$. Since

$$J_{n,m}T^{\max} = -\Delta \quad \text{and} \quad J_{n,m}T^{\min} = -\Delta^0$$

holds, one obtains

PROPOSITION 4.8. *The extension of $T^{\min}$ in $\mathcal{H}$ with $J_{n,m}T(A,B)$ self–adjoint are exactly those $T(A,B)$ for which $-\Delta(A,B)$ is self–adjoint in $\mathcal{H}$.*

As already mentioned, the self–adjoint realizations $-\Delta(A,B)$ of the maximal Laplacian $-\Delta$ are characterized completely, see for example [60].

REMARK 4.9. *Analogous to the case treated in Proposition 4.8 generalizations of the operator*

$$-\operatorname{sign}(x)\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$$

from intervals to metric graphs can be given. One can search for those extensions $-\Delta(A,B)$ of the minimal Laplacian $-\Delta^0$ with $-J_{n,m}\Delta(A,B)$ self–adjoint in $\mathcal{H}$ (or equivalently $-\Delta(A,B)$ Krein space self–adjoint in $\mathfrak{K}$). Analogous to Proposition 4.8 one obtains that the operator $-J_{n,m}\Delta(A,B)$ is self–adjoint in $\mathcal{H}$ if and only if $T(A,B)$ is self–adjoint in $\mathcal{H}$. Consequently these extensions can be characterized using Theorem 4.2. Note that the operator $-\operatorname{sign}(x)\frac{d^2}{dx^2}$ is similar to a self–adjoint operator in the Hilbert space $L^2(\mathbb{R};\mathbb{C})$, see [25], whereas the operator $-\operatorname{sign}(x)\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ is not similar to a self–adjoint operator, compare Example 1.11 in Chapter 1.

In the article [26] the eigenvalue problem is studied for operators of the type $-\operatorname{sign}(x)\frac{d^2}{dx^2}$ on compact finite metric graphs, which have been described here in Proposition 4.8. There the eigenvalues are characterized using variational methods for generalized eigenvalue problems. The application of variational methods to indefinite operators on bounded intervals, generated by expressions of the type $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ is discussed extensively in Chapter 6.

4.2. Indefinite form methods

An approach that has turned out to be very fruitful for sign–definite operators in Hilbert spaces is the one using quadratic forms. Representation theorems give a one–to–one correspondence between closed semi–bounded forms and self–adjoint operators, see for example [58, Chapter VI]. The quadratic form defined by $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ is symmetric, but not semi–bounded. However there are generalizations of the first representation theorem to indefinite quadratic forms. One formulation is given in [43], for further information on indefinite quadratic forms see also the references given therein, in particular the works [38] and [75]. The application of this result to certain indefinite second order differential operators on bounded domains is going to be discussed in the article [56] which is still in preparation. The results obtained there are reproduced and discussed briefly in Chapter 5. An analogous construction can be given for certain compact metric graphs. This approach is outlined in this section and compared to the previously obtained results, where methods from extension theory have been used.

Assume that $(\mathcal{G},\underline{a})$ is a *compact star graph*, that is one has finitely many internal edges $\mathcal{I}$, and the initial vertices of all edges are unified in one vertex and all terminal vertices are vertices of degree one. This means $\partial_-(i_p)=\partial_-(i_q)$ for $i_p,i_q\in\mathcal{I}$ and $\partial_+(i_p)\neq\partial_+(i_q)$, for $i_p\neq i_q$. On the compact star graph $(\mathcal{G},\underline{a})$ one considers the spaces $H^1(\mathcal{G})\subset\mathcal{W}$ and $H^1_0(\mathcal{G})\subset\mathcal{W}$, where

$$H^1(\mathcal{G}):=\{\psi\in\mathcal{W}\mid \psi_j(0)=\psi_i(0),\ i,j\in\mathcal{I}\}$$

and

$$H^1_0(\mathcal{G}):=\left\{\psi\in H^1(\mathcal{G})\mid \psi_j(a_j)=0,\ j\in\mathcal{I}\right\}.$$

Define now the gradient operator in $\mathcal{H}$ by

$$D\colon H^1_0(\mathcal{G})\to\mathcal{H},\quad \psi\mapsto\psi',$$

whose adjoint operator is

$$D^*\colon H^1(\mathcal{G})\to\mathcal{H},\quad \psi\mapsto-\psi'.$$

The operator D and the space $\operatorname{Ran}D$ are closed. The proof is analogous to the one of Lemma 5.1 in Chapter 5 and it can be performed using the Poincaré inequality for $H^1_0(\mathcal{G})$, see Proposition 2.15 in Chapter 2. Since $\operatorname{Ran}D$ is closed, it is itself a Hilbert space with the Hilbert space structure inherited from $\mathcal{H}$. Hence

$$Q\colon\mathcal{H}\to\operatorname{Ran}D,\quad Qu=\begin{cases}u, & u\in\operatorname{Ran}D,\\ 0, & u\perp\operatorname{Ran}D\end{cases}$$

is a partial isometry. The adjoint Q^* is the embedding from $\operatorname{Ran}D$ to $\mathcal{H}$. Note that $(\operatorname{Ran}D)^\perp$ is the space of constant functions in $H^1(\mathcal{G})$. Since Q maps on the orthogonal complement of the constant functions the operator Q becomes more precisely

$$Qu=u-\frac{1}{\sum_{i\in\mathcal{I}}a_i}\int_{\mathcal{G}}u.$$

The operators D and D^* were used implicitly in the article [72] to apply form methods to Laplace operators on finite metric graphs. Here one obtains a graph version of the forthcoming Theorem 5.4.

THEOREM 4.10. *Let* $(\mathcal{G},\underline{a})$ *be a compact star graph and*

(a) $A\in L^\infty(\mathcal{G};\mathbb{R})$*, that is* $A_j\in L^\infty(I_j;\mathbb{R})$*, for each* $j\in\mathcal{I}$*, be such that*

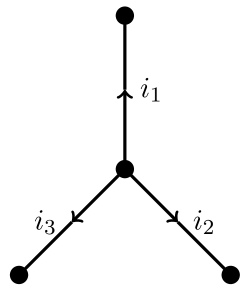


FIGURE 4. A compact star graph with three edges.

(b) *the operator* $QM_AQ^* : \operatorname{Ran} D \to \operatorname{Ran} D$ *is boundedly invertible, where* M_A *is the multiplication operator*

$$M_A \colon \mathcal{H} \to \mathcal{H}, \quad \phi \mapsto A(\cdot)\phi.$$

Then

(i) *there exists a unique self-adjoint operator* $\mathcal{L}$ *with* $\operatorname{Dom}(\mathcal{L}) \subset H_0^1(\mathcal{G})$ *such that*

$$\langle \varphi, \mathcal{L}\psi\rangle_{\mathcal{H}} = \langle \varphi', A(\cdot)\psi'\rangle_{\mathcal{H}}$$

holds for all $\varphi \in H_0^1(\mathcal{G})$ *and all* $\psi \in \operatorname{Dom}(\mathcal{L})$*, and the domain of* $\mathcal{L}$ *is given by*

$$\operatorname{Dom}(\mathcal{L}) = \{\psi \in H_0^1(\mathcal{G}) \mid M_A D\psi \in H^1(\mathcal{G})\}.$$

For any $\psi \in \operatorname{Dom}(\mathcal{L})$ *one has* $\mathcal{L}\psi = D^* M_A D\psi$*, the domain* $\operatorname{Dom}(\mathcal{L})$ *is a core for the gradient operator* D*;*

(ii) *the operator* $\mathcal{L}$ *is boundedly invertible and its inverse* $\mathcal{L}^{-1}$ *is compact. In particular, the spectrum of* $\mathcal{L}$ *is purely discrete.*

The proof of Theorem 4.10 relies on the representation theorem for indefinite quadratic forms [43, Theorem 2.3 and Lemma 2.2]. It is only sketched here for the sake of completeness, since it is completely analogous to the proof appearing in [56], which is due to my co–authors.

SKETCH OF THE PROOF OF THEOREM 4.10. One verifies that the operator $D \colon H_0^1(\mathcal{G}) \to \mathcal{H}$ is boundedly invertible and bounded as map between Hilbert spaces. The kernel of D^* is the space of constant functions in $H^1(\mathcal{G})$ and one has $(\operatorname{Ran} D)^\perp = \operatorname{Ker} D^*$. The operators D and D^* admit the polar decomposition

$$D = U|D| = |D^*|U, \qquad D^* = U^*|D^*| = |D|U^*,$$

where U is a partial isometry with initial subspace $(\operatorname{Ker} D)^\perp = \mathcal{H}$ and final subspace $\operatorname{Ran} D$. One can show that U maps $\operatorname{Dom}(D)$ to $\operatorname{Dom}(D^*) \cap \operatorname{Ran} D$. Furthermore $\operatorname{Ran} D$ is an invariant subspace of DD^*. Note that the operator $-\Delta_N = DD^*$ is the Neumann Laplace operator on $(\mathcal{G}, \underline{a})$ with the so called Kirchhoff or standard boundary conditions at vertices of degree greater one and with Neumann boundary conditions imposed on the vertices of degree one, see [72, Sections 3.2.2 and 3.2.4]. Accordingly one has that the operator $-\Delta_D = D^*D$ is the Dirichlet Laplace operator on $(\mathcal{G}, \underline{a})$ with the so called Kirchhoff or standard boundary conditions at vertices of degree greater one and with Dirichlet boundary conditions imposed on the vertices of degree one, see [72, Sections 3.2.2 and 3.2.4].

Using D and D^* one can adapt the form defined by $\langle\varphi', A(\cdot)\psi'\rangle_{\mathcal{H}}$ to the situation considered in [43, Theorem 2.3]. One considers the auxiliary operator

$$\mathcal{T} = QDD^*Q^*$$

in the Hilbert space $\operatorname{Ran} D$, which is self–adjoint and strictly positive, and the auxiliary form $\mathfrak{b}$ defined by

$$\mathfrak{b}[f,g] = \langle \mathcal{T}^{1/2} f, QM_AQ^*\mathcal{T}^{1/2} g\rangle_{\operatorname{Ran} D}, \qquad f,g \in \operatorname{Dom}(\mathcal{T}^{1/2}) \subset \operatorname{Ran} D.$$

Note that $\mathcal{T}$ is unitarily equivalent to the Dirichlet Laplacian $-\Delta_D$. The crucial condition to apply the representation theorem [43, Theorem 2.3] to the form $\mathfrak{b}$, is that the operator QM_AQ^* in the Hilbert space $\operatorname{Ran} D$ is invertible. Assuming this, the operator

$$B = \mathcal{T}^{1/2} QM_AQ^* \mathcal{T}^{1/2}$$

is the unique self–adjoint operator associated with the form $\mathfrak{b}$ and furthermore the operator B is invertible and has compact inverse. Define by

$$\hat{B}u = \begin{cases} Bu, & u \in \operatorname{Ran} D, \\ 0, & u \perp \operatorname{Ran} D \end{cases}$$

the continuation of B to the whole space $\mathcal{H}$. Using the polar decomposition of D one obtains that

$$\mathcal{L} := U^*\hat{B}U = D^*M_AD$$

and furthermore $\mathcal{L}$ is the unique self–adjoint operator associated to the form defined by $\langle\varphi', A(\cdot)\psi'\rangle_{\mathcal{H}}$. Just as B the operator $\mathcal{L}$ is invertible and has compact inverse. □

PROPOSITION 4.11. *Let $(\mathcal{G}, \underline{a})$ be a compact star graph and let $A(\cdot), A(\cdot)^{-1} \in L^\infty(\mathcal{G};\mathbb{R})$. Then QAQ^* is boundedly invertible if and only if*

$$\int_{\mathcal{G}} \frac{1}{A} \neq 0.$$

The proof is based on the fact that the space $(\operatorname{Ran} D)^\perp = \operatorname{Ker} D^*$ is the one dimensional space of constant functions in $H^1(\mathcal{G})$. It is analogous to the one that is going to be presented in [56] and omitted here. Applying Proposition 4.11 to the function

$$J_{n,m}\colon \mathcal{G} \to \mathbb{C},\ x_j \mapsto \begin{cases} +1, & j \in \mathcal{I}_+, \\ -1, & j \in \mathcal{I}_-, \end{cases}$$

where $\mathcal{I} = \mathcal{I}_+ \dot{\cup} \mathcal{I}_-$ one obtains that $QM_{J_{n,m}}Q^*$ is boundedly invertible if and only if

$$\sum_{i\in\mathcal{I}_+} a_i - \sum_{i\in\mathcal{I}_-} a_i \neq 0.$$

Then by applying Theorem 4.10 one obtains that the form $\mathfrak{l}_{n,m}$ given by

$$\mathfrak{l}_{n,m}[\varphi,\psi] = \langle\varphi', J_{n,m}\psi'\rangle_{\mathcal{H}}, \qquad \varphi,\psi \in H^1_0(\mathcal{G}) \subset \mathcal{H}$$

defines uniquely the operator

$$\mathcal{L}_{n,m} = D^*J_{n,m}D$$

in $\mathcal{H}$ with natural domain $\operatorname{Dom}(\mathcal{L}_{n,m}) \subset H^1_0(\mathcal{G})$. Note that the operator $\mathcal{L}_{n,m}$ is a self–adjoint extension of $T^{\min}$ and therefore there are operators A, B in $\mathcal{K}$ such that $\mathcal{L}_{n,m} = T(A,B)$. More

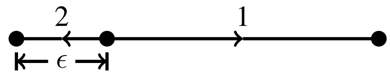


FIGURE 5. The metric graph $(\mathcal{G}, \underline{a}_\epsilon)$ considered in Remark 4.13.

precisely, the operator $T(A,B)$ is defined by Dirichlet boundary conditions on the vertices of degree one and at the central vertex $\nu = \partial_-(i_p)$, $i_p \in \mathcal{I}$, by the local boundary conditions that are given by the matrices

$$A_\nu = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \qquad B_\nu = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & \cdots & 1 & \cdots & -1 & -1 \end{bmatrix},$$

where in the last row of B_ν for each edge in $\mathcal{I}_+$ stands a $+1$ and for each edge in $\mathcal{I}_-$ a -1. To paraphrase, these local boundary conditions guarantee that functions are continuous at the vertices and that the sum of the outward directed derivatives evaluated at the positive incident edges equals the sum of the outward directed derivatives evaluated at the negative incident edges. These local boundary conditions arise naturally from the form approach and therefore they are the main example for self–adjoint boundary conditions discussed here. Note that these boundary conditions are related to the so–called standard or Kirchhoff boundary conditions, compare for example [72, Section 3.2.2] or [63, Example 2.4]. If A_ν^{st} and B_ν^{st} define the standard boundary conditions at the central vertex ν, then one has $A_\nu = A_\nu^{st}$ and $B_\nu = B_\nu^{st} J_{n,m}$. Form methods for indefinite operators with more general matching conditions at the central vertex are not available at present.

REMARK 4.12. *The form approach admits straight forward generalizations to compact graphs, as long as the operator $D\colon H_0^1(\mathcal{G}) \to \mathcal{H}$ is boundedly invertible. This is equivalent to the invertibility of the Dirichlet Laplacian $-\Delta_D = D^*D$. Hence the form approach applies whenever there is at least one vertex of degree one. The obstacle that the form approach cannot be used for arbitrary not necessarily compact finite metric graphs seems to be due to technical difficulties.*

Considering a self–adjoint operator $T(A,B)$ on a metric graph $(\mathcal{G}, \underline{a})$ one can ask the question what is going to happen when shrinking the negative edges' lengths to zero. At this point a general answer to this question cannot be given, but an illustrative example is discussed in the following

REMARK 4.13 (A limit problem). *Consider the operator $T(A,B)$ on the metric graph $(\mathcal{G}, \underline{a}_\epsilon)$ consisting of two internal edges $\mathcal{I}_+ = \{1\}$ and $\mathcal{I}_- = \{2\}$, with lengths $a_1 = 1$ and $a_2(\epsilon) = \epsilon$, $\underline{a}_\epsilon = (a_1, a_2(\epsilon))$, where the self–adjoint boundary conditions are defined by*

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \textit{and} \quad B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

This operator is equivalent to the operator $-\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx}$ *in* $L^2([-\epsilon, 1]; \mathbb{C})$, $\epsilon > 0$ *with Dirichlet boundary conditions imposed at the endpoints. A direct computation shows that for* $\epsilon \to 0$ *the positive eigenvalues of the indefinite operator* $T(A, B)$ *converge to the eigenvalues of the Dirichlet Laplacian on* $L^2([0, 1]; \mathbb{C})$. *The same holds for the corresponding eigenfunctions. A direct computation also exhibits that the negative eigenvalues of* $T(A, B)$ *go to* $-\infty$ *for* $\epsilon \to 0$ *and that the eigenfunctions vanish in limit.*

I suspect that the limit behaviour of $T(A, B)$ *on* $\mathcal{H}_\epsilon$ *for* $\epsilon \to 0$ *admits generalizations to certain indefinite operators on bounded domains, as long as they are associated with the corresponding form.*

4.3. Extension theory background

After performing many explicit calculations, one can make one step back and have a look at the problem from the more general viewpoint of extension theory. Extension theory deals with self–adjoint extensions of closed symmetric operators in separabel Hilbert spaces. Actually it has been the starting point of this work to observe that the operator $T^{\min}$ is a closed symmetric operator with equal deficiency indices.

4.3.1. Classical extension theory. The classical theory describes self–adjoint extensions of closed symmetric operators in terms of unitary mappings between the deficiency spaces, see for example [37] and [92].

Instead of the concrete operator $T^{\min}$, consider now two closed symmetric operators A_+ and A_- in separable Hilbert spaces $\mathcal{H}_+$ and $\mathcal{H}_-$, respectively, each with equal deficiency indices

$$d_+(A_+) = d_-(A_+) \, (\leq \infty), \quad d_+(A_-) = d_-(A_-) \, (\leq \infty),$$

where $d_\pm(A_\pm) = \dim \operatorname{Ker}(A^* \mp i)$. Then one can study two operators

$$T := A_+ \oplus -A_- \quad \text{and} \quad \Delta := A_+ \oplus A_-.$$

Both are closed operators in $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ with equal deficiency indices

$$d_\pm(A) = d_\pm(A_+) + d_\mp(A_-) \quad \text{and} \quad d_\pm(\Delta) = d_\pm(A_+) + d_\pm(A_-).$$

In von Neumann's theory the deficiency spaces

$$N_\pm(z) = \operatorname{Ker}(A_\pm^* - z), \qquad z \in \mathbb{C} \setminus \mathbb{R}$$

are important objects. One considers $N_T(z) := \operatorname{Ker}(T^* - z)$. By construction

$$N_T(z) = \operatorname{Ker} \begin{bmatrix} A_+^* - z & 0 \\ 0 & A_-^* + z \end{bmatrix}$$

and therefore $N_T(z) = N_+(z) \oplus N_-(-z)$, whereas for $N_\Delta(z) = \operatorname{Ker}(\Delta^* - z)$

$$N_\Delta(z) = \operatorname{Ker} \begin{bmatrix} A_+^* - z & 0 \\ 0 & A_-^* - z \end{bmatrix}$$

holds and therefore $N_\Delta(z) = N_+(z) \oplus N_-(z)$. The self–adjoint extensions of T are in one–to–one correspondence to the unitary mappings

$$U' \colon N_T(i) \to N_T(-i).$$

Analogous to the above, the self–adjoint extensions of Δ are in one-to-one correspondence to the unitary mappings

$$U \colon N_\Delta(i) \to N_\Delta(-i).$$

One observes that $N_-(i)$ and $N_-(-i)$ are unitarily equivalent, because A_- is a closed and symmetric operator with equal deficiency indices. Let

$$J\colon N_-(i) \to N_-(-i)$$

be such a unitary equivalence. The relation between unitary mappings U and U' is summarized in the following diagram

$$\begin{array}{ccc} N_T(i) = N_+(i) \oplus N_-(i) & \xrightarrow{\mathbb{1}\oplus J} & N_+(i) \oplus N_-(-i) = N_T(i) \\ {\scriptstyle U}\big\downarrow & & {\scriptstyle U'}\big\downarrow \\ N_\Delta(i) = N_+(-i) \oplus N_-(-i) & \xrightarrow{\mathbb{1}\oplus J} & N_+(-i) \oplus N_-(i) = N_\Delta(i) \end{array}$$

and one reads from this that the relation is a one–to–one correspondence, this means each unitary map U defines uniquely a unitary map U' and vice versa. This in turn gives a one–to–one correspondence between the self–adjoint extensions of Δ and the self–adjoint extensions of T.

4.3.2. Spaces of boundary values. In the context of differential operators the description of self–adjoint extensions in terms of boundary values can be more practical. Following A. N. Kočubeĭ, see [59, Theorem 3], for each symmetric operator X, defined in a separable Hilbert space $\mathcal{H}$, with equal deficiency indices, $d_+(X) = d_-(X) \le \infty$ there exists a Hilbert space $\mathcal{K}$ of dimension $d = d_+(X)$ and linear transformations $\Gamma^1, \Gamma^2\colon \operatorname{Dom}(X^*) \to \mathcal{K}$ with the properties,

(1) for any $\varphi, \psi \in \operatorname{Dom}(X^*)$

$$\langle X^*\varphi, \psi\rangle_{\mathcal{H}} - \langle \varphi, X^*\psi\rangle_{\mathcal{H}} = \langle \Gamma^1\varphi, \Gamma^2\psi\rangle_{\mathcal{K}} - \langle \Gamma^2\varphi, \Gamma^1\psi\rangle_{\mathcal{K}},$$

(2) for any $\kappa_1, \kappa_2 \in K$ there is a $\varphi \in \operatorname{Dom}(A^*)$ such that $\Gamma^1\varphi = \kappa_1$ and $\Gamma^2\varphi = \kappa_2$, and
(3) if $\varphi \in \operatorname{Dom}(X)$, then $\Gamma^1\varphi = \Gamma^2\varphi = 0$.

This can be interpreted as a generalization of Green's formula or simply of integration by parts. The triple $(\mathcal{K}, \Gamma^1, \Gamma^2)$ is called *space of boundary values of* X. The self–adjoint extensions of X are given in terms of unitary mappings U in $\mathcal{K}$, see [59, Theorem 2 and 4]. More precisely, one has that all self–adjoint extensions $\widetilde{X}$ of X are restrictions of X^*, and these are parametrized in terms of U, that is one has $\widetilde{X} = X_U$, where $X_U\psi = X^*\psi$ and

$$\operatorname{Dom}(X_U) = \{\varphi \in \operatorname{Dom}(X^*) \mid (U - \mathbb{1})\Gamma^1\varphi + i(U + \mathbb{1})\Gamma^2\varphi = 0\}.$$

Consider the same situation as above with closed and symmetric operators $A_\pm$ each with equal deficiency indices. Let $(K_\pm, \Gamma^1_\pm, \Gamma^2_\pm)$ be the spaces of boundary values of $A_\pm$. Then the space of boundary values for Δ is given by $(K, \Gamma^1_\Delta, \Gamma^2_\Delta)$ with $K = K_+ \oplus K_-$,

$$\Gamma^1_\Delta = \begin{bmatrix} \Gamma^1_+ & 0 \\ 0 & \Gamma^1_- \end{bmatrix} \quad \text{and} \quad \Gamma^2_\Delta = \begin{bmatrix} \Gamma^2_+ & 0 \\ 0 & \Gamma^2_- \end{bmatrix},$$

which are given with respect to the decomposition $K = K_+ \oplus K_-$. For T the space of boundary values is given then by $(K, \Gamma^1_T, \Gamma^2_T)$, again with $K = K_+ \oplus K_-$, but now with

$$\Gamma^1_T = \begin{bmatrix} \Gamma^1_+ & 0 \\ 0 & \Gamma^1_- \end{bmatrix} \quad \text{and} \quad \Gamma^2_T = \begin{bmatrix} \Gamma^2_+ & 0 \\ 0 & -\Gamma^2_- \end{bmatrix}.$$

As in the parametrization of von Neumann there is a one–to–one correspondence of the self–adjoint extensions of Δ and T. Given a unitary map U in K then Δ_U is the restriction of Δ^* to

$$\mathrm{Dom}(\Delta_U) = \{\varphi \in \mathrm{Dom}(\Delta^*) \mid (U - \mathbb{1})\Gamma^1_\Delta\varphi + i(U + \mathbb{1})\Gamma^2_\Delta\varphi = 0\}.$$

With the same U one obtains the extension of T as a restriction of T^* with domain

$$\mathrm{Dom}(T_U) = \{\psi \in \mathrm{Dom}(T^*) \mid (U - \mathbb{1})\Gamma^1_T\psi + i(U + \mathbb{1})\Gamma^2_T\psi = 0\},$$

where $\mathrm{Dom}(T^*) = \mathrm{Dom}(\Delta^*)$, compare also Remark 4.6.

4.3.3. A radially symmetric example. To come full circle one goes back to the starting point – the differential operator given in (52). Consider the formal differential operator τ in $L^2(\mathbb{R}^2) \equiv L^2(\mathbb{R}^2; \mathbb{C})$ defined by

$$\tau u = -\mathrm{div}\, A(\cdot)\,\mathrm{grad}\, u, \quad A(x) = \begin{cases} +1, & x \in \Omega_+, \\ -1, & x \in \Omega_-, \end{cases}$$

where

$$\begin{aligned} \Omega_+ &= \{x \in \mathbb{R}^2 \mid \|x\| \leq R_1\} \cup \{x \in \mathbb{R}^2 \mid \|x\| \geq R_2\}, \\ \Omega_- &= \{x \in \mathbb{R}^2 \mid R_1 < \|x\| < R_2\} \end{aligned}$$

with $R_2 > R_1 > 0$. This ring geometry has been studied in the article [22]. As $A(\cdot)$ is radially symmetric one can transform the operator τ to polar coordinates. Using the divergence and the gradient operator in polar coordinates one obtains

$$\tau u(r,\theta) = \frac{1}{r}\frac{d}{dr} r A(r) \frac{d}{dr} u(r,\theta) + \frac{1}{r^2} A(r) \frac{d^2}{d\theta^2} u(r,\theta),$$

where

$$A(r) = \begin{cases} +1, & r \in (0, R_1] \cup [R_3, \infty), \\ -1, & r \in (R_2, R_3). \end{cases}$$

Using a separation of variables one obtains that τ is unitarily equivalent to

$$\tilde{\tau} = \bigoplus_{m \in \mathbb{Z}} \tau_m,$$

where τ_m are operators in $L^2(0,\infty)$ defined by

$$\tau_m u_m(r) = -\frac{\partial r}{\partial r} A(r) \frac{\partial r}{\partial r} u_m(r) + A(r) \frac{m^2 - 4^{-1}}{r} u_m(r).$$

Denote by AC_{loc} the set of locally absolutely continuous functions on the interval $(0,\infty)$. The natural (maximal) domain for τ_m in $L^2(0,\infty)$ is

$$\mathrm{Dom}(T_m) = \{u_m \in L^2(0,\infty) \mid u_m, A(\cdot)u_m' \in AC_{loc} \text{and } \tau_m u_m \in L^2(0,\infty)\}$$

for $m \neq 0$ and for $m = 0$ one imposes additionally the assumption (or rather boundary condition)

$$\lim_{r \to 0} [\sqrt{r}\ln(r)]^{-1} u_0(r) = 0.$$

From the general considerations in this section or from the Sturm-Liouville theory, see for example [91], one can deduce that the operators

$$T_m = (\tau_m, \mathrm{Dom}(\tau_m))$$

are self–adjoint. Transforming back one obtains that $T = (\tau, \mathrm{Dom}(T))$ on the natural domain

$$\mathrm{Dom}(T) = \left\{u \in L^2(\mathbb{R}^2) \mid u \in H^1(\mathbb{R}^2), -\mathrm{div}\, A(\cdot)\,\mathrm{grad}\, u \in L^2(\Omega)\right\}$$

is essentially self–adjoint. Observe that $\mathrm{Dom}(T)$ is a subset of $H^1(\mathbb{R}^2)$ and elements $u \in \mathrm{Dom}(T)$ satisfy the matching condition for the normal derivatives at the threshold of Ω_+ and Ω_-

$$\lim_{\epsilon\to 0+} \frac{d}{dr} u(r+\epsilon, \theta) = -\lim_{\epsilon\to 0-} \frac{d}{dr} u(r+\epsilon, \theta),$$

where $(r, \theta) \in \partial\Omega_+ = \partial\Omega_-$.

4.3.4. Outline. The crucial observation of this chapter is that there is a one–to–one correspondence between the parametrization of the self–adjoint realizations of the model operator τ which acts as “plus Laplace” or “minus Laplace” and the parametrization of the self–adjoint realizations of the positive Laplacian. This can be used to distinguish one realization among the set of realizations. This is done in two steps. First one considers the natural self–adjoint realization of the Laplace operator. This is defined by the so called standard or Kirchhoff boundary conditions and it can be parametrized using a unitary map in the deficiency spaces of the minimal Laplacian. Taking now the same unitary map to parametrize the extensions of the model operator τ gives a distinguished self–adjoint extensions of $T^{\min}$. It turns out that this realization is exactly the natural realization of τ, which is also obtained using indefinite quadratic forms. Natural means that the domain of the operator is the natural domain for the composition $-\frac{d}{dx}A(\cdot)\frac{d}{dx}$.

The conjecture is that this holds in more general situations and that this allows to show the essential self–adjointness of sign–indefinite operators of the type $-\mathrm{div}\, A(\cdot)\,\mathrm{grad}$ in their natural domain in $L^2(\Omega)$ with $A(x)$ elliptic for $x \in \Omega_+$ and $-A(x)$ elliptic for $x \in \Omega_-$, where $\Omega = \Omega_+ \cup \Omega_-$. In a very particular radially symmetric situation this has been verified. The scheme presented here at least gives a distinguished self–adjoint realization of such operators and for the model problem with finite deficiency indices the conjecture is indeed true.

It constitutes an open problem whether the sign–indefinite operators that are considered in this chapter arise naturally as limits of certain operators on “thick graphs” when shrinking the “thickness” to zero. For Laplacians on graphs there are such results, see [36, 41] and the references therein. For Laplace operators on twisted tubes similar results have been obtained recently, see [70]. In particular it has been shown there, that the limit of such operators yields certain Schrödinger operators on the real line.

4.4. Eigenvalues, resonances and resolvents

The study of the spectral resolution of the self–adjoint operator $T(A, B)$ is based on finding solutions of $(\tau - k^2)u(\cdot, k) = 0$ which satisfy the boundary conditions along with certain integrability conditions. Considering each edge separately, one recalls that a fundamental system of the equation

$$-u''(x, k) = k^2 u(x, k) \quad \text{with} \quad k \neq 0, \tag{55}$$

$u\colon \mathbb{R} \to \mathbb{C}$ is given by e^{ikx} and e^{-ikx} and consequently of

$$u''(x,\kappa) = \kappa^2 u(x,\kappa), \quad \text{for} \quad \kappa \neq 0, \tag{56}$$

by $e^{-\kappa x}$ and $e^{\kappa x}$. As the two fundamental systems have different integrability properties in certain regions of $\mathbb{C}$, one defines the two open quadrants

$$\mathcal{Q} = \{k \in \mathbb{C} \mid \mathrm{Re}\,(k) > 0 \text{ and } \mathrm{Im}\,(k) > 0\}$$

and

$$\mathcal{P} = \{k \in \mathbb{C} \mid \mathrm{Re}\,(k) < 0 \text{ and } \mathrm{Im}\,(k) > 0\}.$$

For $k, \kappa \in \mathcal{Q}$ the functions e^{ikx} and $e^{-\kappa x}$ are elements of $L^2([0,\infty);\mathbb{C})$, whereas e^{-ikx} and $e^{\kappa x}$ are not in $L^2([0,\infty);\mathbb{C})$. For $k, \kappa, \in \mathcal{P}$ the functions e^{ikx} and $e^{\kappa x}$ are square integrable on $(0,\infty)$.

4.4.1. Resonances and non–zero eigenvalues. A general *Ansatz* for a solution that satisfies simultaneously equation (55) on the positive edges and equation (56) on the negative edges is the function ψ defined by

$$\psi(x,k,i\kappa) = \begin{cases} s_j(k) e^{ikx_j}, & j \in \mathcal{E}_+, \\ \alpha_j(k) e^{ikx_j} + \beta_j(k) e^{-ikx_j}, & j \in \mathcal{I}_+, \\ s_j(i\kappa) e^{-\kappa x_j}, & j \in \mathcal{E}_-, \\ \alpha_j(i\kappa) e^{-\kappa x_j} + \beta_j(i\kappa) e^{\kappa x_j}, & j \in \mathcal{I}_- \end{cases} \tag{57}$$

with $k, \kappa \in \mathbb{C} \setminus \{0\}$ and appropriate coefficients $s_j(k), \alpha_j(k), \beta_j(k)$ and $s_j(i\kappa), \alpha_j(i\kappa), \beta_j(i\kappa)$. With this notation one has

$$(\tau - k^2)\psi(x,k,\pm ik) = 0 \quad \text{and} \quad (-\Delta - k^2)\psi(x,k,\pm k) = 0.$$

Assuming that $\mathcal{E}_-, \mathcal{E}_+ \neq \emptyset$ one has for $k \in \mathcal{Q}$, that $\psi(\cdot,k,ik)$ is square integrable. Analogous for $k \in \mathcal{P}$, $\psi(\cdot,k,-ik)$ is square integrable on the external edges, as now $e^{kx} \in L^2([0,\infty);\mathbb{C})$. Introduce for brevity the notations

$$\chi_+(k) = \begin{bmatrix} \{s_j(k)\}_{j\in\mathcal{E}_+} \\ \{\alpha_j(k)\}_{j\in\mathcal{I}_+} \\ \{\beta_j(k)\}_{j\in\mathcal{I}_+} \end{bmatrix}, \qquad \chi_-(i\kappa) = \begin{bmatrix} \{s_j(i\kappa)\}_{j\in\mathcal{E}_-} \\ \{\alpha_j(i\kappa)\}_{j\in\mathcal{I}_-} \\ \{\beta_j(i\kappa)\}_{j\in\mathcal{I}_-} \end{bmatrix}$$

and

$$\chi(k,i\kappa) = \begin{bmatrix} \chi_+(k) \\ \chi_-(i\kappa) \end{bmatrix}.$$

For the boundary values of the *Ansatz* function $\psi(\cdot,k,i\kappa)$ one obtains the formulae

$$\underline{\psi(\cdot,k,i\kappa)} = X_{n,m}(k,i\kappa,\underline{a})\chi(k,ik), \qquad \underline{\psi(\cdot,k,i\kappa)'} = Y_{n,m}(k,i\kappa,\underline{a})\chi(k,ik),$$

where

$$X_{n,m}(k,i\kappa,\underline{a}) = \begin{bmatrix} X_n(k,\underline{a}_+) & 0 \\ 0 & X_m(i\kappa,\underline{a}_-) \end{bmatrix}$$

and

$$Y_{n,m}(k,i\kappa,\underline{a}) = \begin{bmatrix} Y_n(k,\underline{a}_+) & 0 \\ 0 & Y_m(i\kappa,\underline{a}_-) \end{bmatrix}$$

are matrices in $\mathcal{K}$, which are written with respect to the decomposition $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$. This uses the notation

$$X_l(k,\underline{b}) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & \mathbb{1} \\ 0 & e^{ik\underline{b}} & e^{-ik\underline{b}} \end{bmatrix} \quad \text{and} \quad Y_l(k,\underline{b}) = ik \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & -\mathbb{1} \\ 0 & e^{ik\underline{b}} & -e^{ik\underline{b}} \end{bmatrix},$$

where for $l = n$ one has to plug in $\underline{b} = \underline{a}_+$ and for $l = m$ one inserts $\underline{b} = \underline{a}_-$. Actually these are the matrices known from the spectral theory of Laplace operators on $(\mathcal{G}_+, \underline{a}_+)$ and $(\mathcal{G}_-, \underline{a}_-)$, see for example [63, Section 3]. The matrices $X_n(k, \underline{a}_+)$ and $Y_n(k, \underline{a}_+)$ define operators in $\mathcal{K}_+$, and $X_m(k, \underline{a}_-)$ and $Y_m(k, \underline{a}_-)$ in $\mathcal{K}_-$, respectively. Recall that $e^{ik\underline{b}}$ denotes the diagonal matrix with entries $\{e^{ik\underline{b}}\}_{k,l} = \delta_{k,l} e^{ikb_l}$, where $b_l \in \underline{b}$ and $\delta_{k,l}$ denotes the Kronecker delta.

Note that there is a function $\psi(\cdot, k, i\kappa)$ of the form (57) satisfying the boundary conditions $A\underline{\psi(\cdot, k, i\kappa)} + B\underline{\psi(\cdot, k, i\kappa)'} = 0$, if and only if there exist coefficients $\chi(k, i\kappa) \in \mathcal{K} \setminus \{0\}$ such that

$$Z_{n,m}(A, B, k, i\kappa, \underline{a})\chi(k, i\kappa) = 0 \tag{58}$$

holds with

$$Z_{n,m}(A, B, k, i\kappa, \underline{a}) = AX_{n,m}(k, i\kappa, \underline{a}) + BY_{n,m}(k, i\kappa, \underline{a}).$$

Since $\mathcal{K}$ is a finite dimensional space the condition

$$\det Z_{n,m}(A, B, k, i\kappa, \underline{a}) = 0$$

is equivalent to the condition given in equation (58).

REMARK 4.14. *Let $T(A,B)$ be self-adjoint. Then there are no $\psi(\cdot, k, ik)$ of the form* (57)*, for $k \in \mathcal{Q}$ with $(\tau - k^2)\psi(\cdot, k, ik) = 0$ and $\psi(\cdot, k, ik) \in \mathrm{Dom}(T(A,B))$. Similarly for $k \in \mathcal{P}$, there is no such $\psi(\cdot, k, -ik)$ with $(\tau - k^2)\psi(\cdot, k, -ik) = 0$ that satisfies $\psi(\cdot, k, -ik) \in \mathrm{Dom}(T(A,B))$. This is due to the fact that $\psi(\cdot, k, ik)$ and $\psi(\cdot, k, -ik)$, respectively would be square integrable eigenfunctions to the complex eigenvalue k^2, which would contradict the self–adjointness of $T(A,B)$. The question at which points the resolvent $R(k^2) = (T(A,B) - k^2)^{-1}$ as function in k admits a meromorphic continuation to the real line is related to equation* (58)*. The poles of the meromorphic continuation of $R(\cdot)$ are linked to certain singular points of $Z_{n,m}(A, B, \cdot, \cdot, \underline{a})$.*

For star graphs, that is for graphs with $\mathcal{I} = \emptyset$, the matrix $Z_{n,m}(A, B, k, i\kappa)$ simplifies to become

$$Z_{n,m}(A, B, k, i\kappa) = A + B \begin{bmatrix} ik & 0 \\ 0 & -\kappa \end{bmatrix}.$$

Instead of the matrices A, B one can consider the equivalent parametrization according to Corollary 4.5. There is an orthogonal projector P and a Hermitian matrix L acting in $\operatorname{Ker} P$ such that with $A' = L + P$ and $B' = P^{\perp} J_{n,m}$ one has $T(A', B') = T(A, B)$. Denote by l_j the eigenvalues of L and by P_j the orthogonal projector on the corresponding eigenspace. Then one has for $k, \kappa \in \mathbb{C} \setminus \{0\}$ the representation

$$Z_{n,m}(A, B, k, i\kappa) = P + \sum_j P_j \left(l_j + \begin{bmatrix} -ik & 0 \\ 0 & \kappa \end{bmatrix} \right).$$

Analogous to [60, Theorem 3.1] one proves now

LEMMA 4.15. *Let $T(A,B)$ be self–adjoint. Then the zeros of the function*

$$k \mapsto \det Z_{n,m}(A,B,k,ik,\underline{a})$$

are discrete and there are no zeros in $\mathcal{Q}$. For $\mathcal{I} = \emptyset$ there are $|\mathcal{E}|$ zeros in $\overline{\mathcal{Q}}$ at the most. The analogous statements hold for the zeros of $\kappa \mapsto \det Z_{n,m}(A,B,i\kappa,\kappa,\underline{a})$.

PROOF. The function $k \mapsto \det Z_{n,m}(A,B,k,ik,\underline{a})$ is an entire function. This follows directly from the definition. Therefore it can be represented as a power series. If the zeros had not been discrete, then there would be a convergent sequence $\{k_j\}_{j\in\mathbb{N}}$ such that $\det Z_{n,m}(A,B,k_j,ik_j,\underline{a}) = 0$. This would imply that $\det Z_{n,m}(A,B,k,ik,\underline{a}) \equiv 0$. Therefore it is sufficient to find one point $k_0 \in \mathbb{C}$ for which $\det Z_{n,m}(A,B,k_0,ik_0,\underline{a}) \neq 0$. If there had been such a k_0 with $\det Z_{n,m}(A,B,k_0,ik_0,\underline{a}) = 0$ from the open quadrant $\mathcal{Q}$, this would imply the integrability of the *Ansatz* function $\psi(x,k_0,ik_0)$. According to Remark 4.14 then $k_0^2 \notin \mathbb{R}$ would be an eigenvalue of $T(A,B)$, which is a contradiction to the self–adjointness of $T(A,B)$. □

Putting the pieces together one obtains

PROPOSITION 4.16. *Let $T(A,B)$ be self–adjoint. Then $k^2 > 0$ is an eigenvalue of $T(A,B)$ if and only if there is a coefficient $\chi(k,ik) \neq 0$ with $s_j(k) = 0$ for $j \in \mathcal{E}_+$ and for the positive square roots $k > 0$ of k^2 such that*

$$Z_{n,m}(A,B,k,ik,\underline{a})\chi(k,ik) = 0.$$

The number $-\kappa^2 < 0$ is a negative eigenvalue of $T(A,B)$ if and only if for the positive square root $\kappa > 0$ of κ^2 there is a coefficient $\chi(i\kappa,\kappa) \neq 0$ with $s_j(\kappa) = 0$ for $j \in \mathcal{E}_-$ such that

$$Z_{n,m}(A,B,i\kappa,\kappa,\underline{a})\chi(i\kappa,\kappa) = 0 \quad \textit{with} \quad s_j(\kappa) = 0.$$

In particular for $\mathcal{E} = \emptyset$ one obtains

COROLLARY 4.17. *Let $T(A,B)$ be self-adjoint and assume that $\mathcal{E} = \emptyset$. Then the positive square roots $k > 0$ of positive eigenvalues k^2 are exactly the solutions of the secular equation*

$$\det Z_{n,m}(A,B,k,ik,\underline{a}) = 0$$

and the positive square roots $\kappa > 0$ of the absolute values of negative eigenvalues $-\kappa^2$ are exactly the solutions of the secular equation

$$\det Z_{n,m}(A,B,i\kappa,\kappa,\underline{a}) = 0.$$

REMARK 4.18. *In the presence of external edges only the solutions that are square integrable on the external edges are eigenvalues. In general one cannot exclude other resonances in the set of singular points of the function $k \mapsto Z_{n,m}(A,B,k,ik,\underline{a})$. In all the examples I have studied the resonances were only the eigenvalues, but I have not been able to find a general proof.*

4.4.2. Eigenvalue zero. The solutions of

$$u''(x) = 0$$

are the affine functions and only the trivial solution is square integrable on $[0,\infty)$. Thus one gets to the *Ansatz*

$$\psi^0(x) = \begin{cases} 0, & j \in \mathcal{E}_+ \cup \mathcal{E}_-, \\ \alpha_j^0 + \beta_j^0 x_j, & j \in \mathcal{I}_+ \cup \mathcal{I}_-, \end{cases}$$

for appropriate coefficients α_j^0, β_j^0. The coefficients appearing on the right hand side are written into the vectors

$$\chi_+^0 = \begin{bmatrix} 0 \\ \{\alpha_j^0\}_{j\in\mathcal{I}_+} \\ \{\beta_j^0\}_{j\in\mathcal{I}_+} \end{bmatrix} \quad \text{and} \quad \chi_-^0 = \begin{bmatrix} 0 \\ \{\alpha_j^0\}_{j\in\mathcal{I}_-} \\ \{\beta_j^0\}_{j\in\mathcal{I}_-} \end{bmatrix}, \tag{59}$$

which are summarized in one vector

$$\chi^0 = \begin{bmatrix} \chi_+^0 \\ \chi_-^0 \end{bmatrix}.$$

For the boundary values one obtains

$$\underline{\psi^0} = X_{n,m}^0(\underline{a})\chi^0 \quad \text{and} \quad \underline{\psi^{0\prime}} = Y_{n,m}^0(\underline{a})\chi^0$$

with

$$X_{n,m}^0(\underline{a}) = \begin{bmatrix} X_n^0(\underline{a}_+) & 0 \\ 0 & X_m^0(\underline{a}_-) \end{bmatrix} \quad \text{and} \quad Y_{n,m}^0(\underline{a}) = \begin{bmatrix} Y_n^0(\underline{a}_+) & 0 \\ 0 & Y_m^0(\underline{a}_-) \end{bmatrix},$$

which are matrices in $\mathcal{K}$, that are written with respect to the decomposition $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$. This uses the notation

$$X_l^0(\underline{b}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & \mathbb{1} & \underline{b} \end{bmatrix} \quad \text{and} \quad Y_l^0(\underline{b}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathbb{1} \\ 0 & 0 & -\mathbb{1} \end{bmatrix},$$

where for $l = n$ one has to plug in $\underline{b} = \underline{a}_+$ and for $l = m$ one inserts $\underline{b} = \underline{a}_-$. Actually these are the matrices known from the spectral theory of Laplace operators on finite metric graphs, compare Section 2.3 of Chapter 2. The matrices $X_n^0(\underline{a}_+)$ and $Y_n^0(\underline{a}_+)$ define operators in $\mathcal{K}_+$, and the matrices $X_m^0(\underline{a}_-)$ and $Y_m^0(\underline{a}_-)$ define operators in $\mathcal{K}_-$. Recall that $\underline{b}$ denotes the diagonal matrix with entries $\{\underline{b}\}_{k,l} = \delta_{k,l} b_l$. This gives

PROPOSITION 4.19. *In the presence of external edges, zero is an eigenvalue of $T(A,B)$ if and only if there exists a vector χ^0 with entries of the form* (59) *such that*

$$(AX_{n,m}^0(\underline{a}) + BY_{n,m}^0(\underline{a}))\chi^0 = 0.$$

Let $\mathcal{E} = \emptyset$. Then zero is an eigenvalue of $T(A,B)$ if and only if

$$\det(AX_{n,m}^0(\underline{a}) + BY_{n,m}^0(\underline{a})) = 0,$$

and the dimension of $\operatorname{Ker} T(A,B)$ *is equal to the dimension of* $\operatorname{Ker}(AX_{n,m}^0(\underline{a}) + BY_{n,m}^0(\underline{a}))$.

REMARK 4.20. *Since the solutions of $u''(x) = 0$ are affine functions one can use the same Ansatz ψ^0 to find solutions of the Laplace equation $\Delta u = 0$ on the graph. Consequently zero is an eigenvalue of $T(A,B)$ if and only if zero is an eigenvalue of the not necessarily self–adjoint Laplace operator $-\Delta(A,B)$. Note that $-\Delta(A,B)$ has the same domain as $T(A,B)$, since it is defined by the same boundary conditions.*

4.4.3. Eigenvalue asymptotics. Assume $T(A,B)$ to be self–adjoint, then its eigenvalues, according to Lemma 4.15, are discrete with only finite multiplicities. Denote by

$$0 < \lambda_1^+ \leq \lambda_2^+ \leq \dots$$

the positive eigenvalues, counted with multiplicities and by

$$0 > -\lambda_1^- \geq -\lambda_2^- \geq \dots$$

the negative eigenvalues, counted with multiplicities. Note that in general, the eigenvalues of $T(A,B)$ can be embedded in the continuous spectrum. One defines the counting function for the positive eigenvalues $N_+(\cdot; T(A,B))$ and the counting function for the negative eigenvalues $N_-(\cdot; T(A,B))$ by

$$N_\pm(\lambda; T(A,B)) = \sum_{\lambda_j^\pm < \lambda} 1.$$

In certain cases a generalized Weyl law holds for the asymptotic behaviour of the eigenvalue counting functions.

PROPOSITION 4.21.

(1) Assume that $(\mathcal{G}, \underline{a})$ is a compact metric graph, that is $\mathcal{E} = \emptyset$, and let $T(A,B)$ be self-adjoint. Then asymptotically the eigenvalue counting functions are

$$N_\pm(\lambda; T(A,B)) \sim \frac{1}{\pi}\left(\sum_{i\in\mathcal{I}_\pm} a_i\right)\lambda^{1/2}, \textit{ for } \lambda \to \infty.$$

(2) Assume that $(\mathcal{G}, \underline{a})$ is non–compact, but $\mathcal{E}_- = \emptyset$ $(\mathcal{E}_+ = \emptyset)$ and let $T(A,B)$ be self-adjoint. Then the asymptotic formula for $N_-(\lambda; T(A,B))$ $(N_+(\lambda; T(A,B)))$ still holds.

PROOF. Suppose that $\mathcal{E} = \emptyset$. Then it follows from the compact embedding of $\mathcal{D} \hookrightarrow \mathcal{H}$, compare for example [4, Theorem A 5.4], that $T(A,B)$ has compact resolvent and therefore there exists $k^2 \in \mathbb{R}$ with $k^2 \in \rho(T(A,B)) \cap \rho(T(\mathbb{1},0))$. According to the forthcoming Proposition 4.26, the difference

$$(T(A,B) - k^2)^{-1} - (T(\mathbb{1},0) - k^2)^{-1}$$

is a self-adjoint finite rank operator. To prove the first statement, one applies the $\min - \max$–principle to the resolvents. As the difference is only finite rank one obtains that

$$N_\pm(\lambda; T(A,B)) \sim N_\pm(\lambda; T(\mathbb{1},0)), \text{ for } \lambda \to \infty,$$

see for example [17, Lemma 1.4]. The operator $T(\mathbb{1},0)$ decouples all edges and defines (positive) Dirichlet Laplacians on each positive edge and Dirichlet Laplacians multiplied with minus one on each negative edge. The claim follows by summing up the eigenvalue counting functions of the Dirichlet Laplacians on the intervals.

To prove the second statement one takes into account that for a bounded operator one can apply the $\min - \max$–principle to characterize the discrete spectrum below the essential spectrum, see for example [34] and the references therein. For the case of $\mathcal{E}_+ \neq \emptyset$ and $\mathcal{E}_- = \emptyset$ the essential spectrum of $T(A,B)$ is $[0,\infty)$ and the negative spectrum is discrete. Denote by

$-\mu_1^- < 0$ the largest negative eigenvalue of $T(\mathbb{1},0)$. Then all $-k^2 \in \big(\max\{-\lambda_1^-, -\mu_1^-\}, 0\big)$ are in the resolvent set of both $T(A,B)$ and $T(\mathbb{1},0)$. For such a $-k^2$ the difference

$$(T(A,B)+k^2)^{-1} - (T(\mathbb{1},0)+k^2)^{-1}$$

is a self-adjoint finite rank operator and the negative spectrum of $(T(A,B)+k^2)^{-1}$ consists of a sequence of eigenvalues of finite multiplicities that accumulate at zero. Therefore one can apply the $\min-\max$–principle to characterize the positive eigenvalues of $-(T(A,B)+k^2)^{-1}$ as well as the positive eigenvalues of $-(T(\mathbb{1},0)+k^2)^{-1}$. As one has again only a perturbation of finite rank the claim follows by the same reasoning as above. □

REMARK 4.22. *For this proof of Proposition 4.21 it is essential to consider only finite rank perturbations. However if the form approach elaborated in Section 4.2 applies and the operator $T(A,B)$ is the operator defined in Theorem 4.10, then one can certainly give a variational characterization of the eigenvalues of $T(A,B)$ on the lines of Proposition 6.1 in Chapter 6. Let $(\mathcal{G},\underline{a})$ be a compact finite metric graph and assume that $T(A,B)$ is self–adjoint and invertible. Then the operator $T(A,B)$ has a compact inverse and the eigenvalues of $T(A,B)^{-1}$ can be determined as the successive extrema of the Rayleigh-quotient*

$$\rho[\psi] := \frac{\langle \tau\psi, \psi\rangle}{\langle \tau\psi, \tau\psi\rangle}, \quad \psi \in \operatorname{Dom}(T(A,B)).$$

This delivers a variational characterizations of the eigenvalues of $T(A,B)$ which can be used to give an alternative proof for the first statement of Proposition 4.21 on the lines of Theorem 6.6 in Chapter 6.

4.4.4. Generalized eigenfunctions. An important tool for the study of the absolutely continuous part of operators $T(A,B)$ and hence for their scattering theory are generalized eigenfunctions. Assume that $\mathcal{E} \neq \emptyset$. For $l \in \mathcal{E}_+$ one *Ansatz* for a generalized eigenfunction is

$$\varphi_l(x,k,i\kappa) = \begin{cases} \delta_{lj}e^{-ikx_l} + s_{lj}(k)e^{ikx_l}, & j \in \mathcal{E}_+, \\ \alpha_{lj}(k)e^{ikx_j} + \beta_{lj}(k)e^{-ikx_j}, & j \in \mathcal{I}_+, \\ s_{lj}(i\kappa)e^{-\kappa x_j}, & j \in \mathcal{E}_-, \\ \alpha_{lj}(i\kappa)e^{-\kappa x_j} + \beta_{lj}(i\kappa)e^{\kappa x_j}, & j \in \mathcal{I}_- \end{cases}$$

and for $l \in \mathcal{E}_-$

$$\varphi_l(x,k,i\kappa) = \begin{cases} s_{lj}(k)e^{ikx_l}, & j \in \mathcal{E}_+, \\ \alpha_{lj}(k)e^{ikx_j} + \beta_{lj}(k)e^{-ikx_j}, & j \in \mathcal{I}_+, \\ \delta_{lj}e^{\kappa x_j} + s_{lj}(i\kappa)e^{-\kappa x_j}, & j \in \mathcal{E}_-, \\ \alpha_{lj}(i\kappa)e^{-\kappa x_j} + \beta_{lj}(i\kappa)e^{\kappa x_j}, & j \in \mathcal{I}_- \end{cases}$$

with δ_{lj} the Kronecker delta and sought after coefficients $s_{lj}(k), \alpha_{lj}(k)$ and $\beta_{lj}(k)$. The functions $\varphi_l(x,k,i\kappa)$, $l \in \mathcal{E}$, are solutions of equation (55) on the positive edges and of equation (56) on the negative edges, but they are not square integrable. For notational simplicity these *Ansatz* functions are written into the $|\mathcal{E}| \times |\mathcal{E} \cup \mathcal{I}|$–matrix valued function $\varphi(x,k,i\kappa)$ with entries

$$\{\varphi(x,k,i\kappa)\}_{lj} := \{\varphi_l(x,k,i\kappa)\}_j\,,$$

that is the (l, j)-th entry of $\varphi(\cdot, k, i\kappa)$ is the restriction of φ_l, $l \in \mathcal{E}$ to I_j, $j \in \mathcal{E} \cup \mathcal{I}$. The coefficients for $l \in \mathcal{E}_+$ are written into the vectors

$$\chi_{l,+}(k) = \begin{bmatrix} \{\delta_{lj} + s_{lj}(k)\}_{j\in\mathcal{E}_+} \\ \{\alpha_{lj}(k)\}_{j\in\mathcal{I}_+} \\ \{\beta_{lj}(k)\}_{j\in\mathcal{I}_+} \end{bmatrix}, \qquad \chi_{l,-}(i\kappa) = \begin{bmatrix} \{s_{lj}(i\kappa)\}_{j\in\mathcal{E}_-} \\ \{\alpha_{lj}(i\kappa)\}_{j\in\mathcal{I}_-} \\ \{\beta_{lj}(i\kappa)\}_{j\in\mathcal{I}_-} \end{bmatrix}$$

and for $l \in \mathcal{E}_-$ into

$$\chi_{l,+}(k) = \begin{bmatrix} \{s_{lj}(k)\}_{j\in\mathcal{E}_+} \\ \{\alpha_j(k)\}_{j\in\mathcal{I}_+} \\ \{\beta_j(k)\}_{j\in\mathcal{I}_+} \end{bmatrix}, \qquad \chi_{l,-}(i\kappa) = \begin{bmatrix} \{\delta_{lj} + s_j(i\kappa)\}_{j\in\mathcal{E}_-} \\ \{\alpha_j(i\kappa)\}_{j\in\mathcal{I}_-} \\ \{\beta_j(i\kappa)\}_{j\in\mathcal{I}_-} \end{bmatrix}.$$

Finally one sets

$$\chi_l(k, i\kappa) = \begin{bmatrix} \chi_{l,+}(k) \\ \chi_{l,-}(i\kappa) \end{bmatrix},$$

which is a vector in $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$. These χ_l, $l \in \mathcal{E}$, are summarized into the $|\mathcal{E}| \times |\mathcal{E} \cup \mathcal{I}|$ matrix $\chi(k, i\kappa)$ with entries

$$\{\chi(k, i\kappa)\}_{lj} := \{\chi_l(k, i\kappa)\}_j .$$

For the boundary values of the *Ansatz* functions $\varphi_l(\cdot, k, i\kappa)$ defined above one obtains the formulae

$$\begin{aligned} \underline{\varphi(\cdot, k, i\kappa)} &= \mathbb{1}_{n+m} e_{n,m} + X_{n,m}(k, i\kappa, \underline{a})\chi(k, i\kappa), \\ \underline{\varphi(\cdot, k, i\kappa)'} &= I_{n,m}(-k, -i\kappa)e_{n,m} + Y_{n,m}(k, i\kappa, \underline{a})\chi(k, i\kappa), \end{aligned}$$

where for brevity

$$I_{n,m}(k, i\kappa) = \begin{bmatrix} ik\mathbb{1}_n & 0 \\ 0 & -\kappa\mathbb{1}_m \end{bmatrix}, \qquad I_{n,m} = \begin{bmatrix} \mathbb{1}_n & 0 \\ 0 & i\mathbb{1}_m \end{bmatrix},$$

which are related by $ik \cdot I_{n,m} = I_{n,m}(k, ik)$. The notation

$$e_{n,m} = \begin{bmatrix} e_n & 0 \\ 0 & e_m \end{bmatrix}, \quad \text{where} \quad e_p = \begin{bmatrix} \mathbb{1} \\ 0 \\ 0 \end{bmatrix}, \quad p \in \{n, m\}$$

is used, where e_n is a $|\mathcal{K}_{\mathcal{E}_+}| \times |\mathcal{K}|$-matrix, e_m a $|\mathcal{K}_{\mathcal{E}_-}| \times |\mathcal{K}|$–matrix and consequently the block operator matrix $e_{n,m}$ is a $\big(|\mathcal{K}_{\mathcal{E}_+}| + |\mathcal{K}_{\mathcal{E}_-}|\big) \times |\mathcal{K}|$–matrix. The boundary conditions

$$A\underline{\varphi_l(\cdot, k, i\kappa)} + B\underline{\varphi_l(\cdot, k, i\kappa)'} = 0, \quad \text{for } l \in \mathcal{E}$$

are satisfied for all $l \in \mathcal{E}$ if and only if

$$(AX_{n,m}(k, i\kappa, \underline{a}) + BY_{n,m}(k, i\kappa, \underline{a}))\chi(k, i\kappa) = -(A\mathbb{1}_{n+m} + BI_{n,m}(-k, -i\kappa))e_{n,m}$$

holds for the coefficient matrix $\chi(k, i\kappa)$. If $AX_{n,m}(k, i\kappa, \underline{a}) + BY_{n,m}(k, i\kappa, \underline{a})$ is invertible one can define the matrix valued transform

$$\mathfrak{X}(k, i\kappa) = -(AX_{n,m}(k, i\kappa, \underline{a}) + BY_{n,m}(k, i\kappa, \underline{a}))^{-1}(A\mathbb{1}_{n+m} + BI_{n,m}(-k, -i\kappa)).$$

This is a transform in A and B as well as in k, κ, but here in the notation the dependence on A and B is omitted. When $\mathfrak{X}(k, i\kappa)$ is well-defined one can solve the equation for the coefficients $\chi(k, i\kappa)$, which are then uniquely determined by

$$\chi(k, i\kappa) = \mathfrak{X}(k, i\kappa) e_{n,m}. \tag{60}$$

Note that $\chi(\pm k, ik)$ is well–defined for all $k > 0$, except the resonances with $\det Z_{n,m}(A, B, \pm k, ik, \underline{a}) = 0$. With the coefficients $\chi(\pm k, ik)$, where $k > 0$ such that $Z_{n,m}(A, B, \pm k, ik, \underline{a})$ is regular, the functions

$$\varphi_l(\cdot, k, ik) \quad \text{and} \quad \varphi_l(\cdot, -k, ik), \quad l \in \mathcal{E}_+,$$

satisfy the boundary conditions $A\underline{\varphi} + B\underline{\varphi_l}' = 0$. By construction they additionally solve the equation $\left(\tau - k^2\right)\varphi = 0$. Therefore, they are denoted *generalized eigenfunctions of* $T(A, B)$ *for positive energies*. Analogous, for $l \in \mathcal{E}_-$ and $\kappa > 0$ such that $Z_{n,m}(A, B, i\kappa, \pm\kappa, \underline{a})$ is regular the functions

$$\varphi_l(\cdot, i\kappa, \kappa) \quad \text{and} \quad \varphi_l(\cdot, i\kappa, -\kappa)$$

are denoted *generalized eigenfunctions of* $T(A, B)$ *for negative energies*. These statements are going to be specified, when considering scattering problems related to the operator $T(A, B)$ in Section 4.5. There the associated wave operators are computed in terms of the generalized eigenfunctions of $T(A, B)$.

4.4.5. Coefficient matrix. For a star graph, that is for $\mathcal{I} = \emptyset$, the coefficients of the generalized eigenfunctions are simplified to become

$$\chi(k, i\kappa) = -(A + BI_{n,m}(k, i\kappa))^{-1}(A + BI_{n,m}(-k, -i\kappa)).$$

Given an arbitrary finite metric graph $(\mathcal{G}, \underline{a})$ and self–adjoint boundary conditions parametrized by matrices A and B one can cut all internal edges in twain and substitute each of the pieces by an external edge. Then the graph becomes a union of star graphs, on which A and B still define a self–adjoint operator. This motivates the definition of the *local coefficient matrix of the generalized eigenfunctions* $\mathfrak{C}(k, i\kappa)$ for any graph and fixed A, B satisfying the assumptions of Theorem 4.2 by

$$\mathfrak{C}(k, i\kappa) := -(A + BI_{n,m}(k, i\kappa))^{-1}(A + BI_{n,m}(-k, -i\kappa)). \tag{61}$$

In short $\mathfrak{C}(k, i\kappa)$ is denoted the *coefficient matrix*. For star graphs $\mathfrak{C}(k, i\kappa) = \mathfrak{X}(k, i\kappa) = \chi(k, i\kappa)$ holds. The coefficient matrix is the analogon of the local scattering matrix

$$\mathfrak{S}(k; A_0, B_0) = -(A_0 + ikB_0)^{-1}(A_0 - ikB_0)$$

that appears in the context of semi–bounded self–adjoint Laplacians $-\Delta(A_0, B_0)$ on metric graphs, see for example [60] or [62], and in the case $\mathcal{E}_- = \emptyset$ both objects coincide. With respect to the block decomposition induced by $\mathcal{E}_+ \cup \mathcal{I}_+$ and $\mathcal{E}_- \cup \mathcal{I}_-$ the coefficient matrix can be written as block operator matrix

$$\mathfrak{C}(k, i\kappa) = \begin{bmatrix} \mathfrak{C}_{++}(k, i\kappa) & \mathfrak{C}_{+-}(k, i\kappa) \\ \mathfrak{C}_{-+}(k, i\kappa) & \mathfrak{C}_{--}(k, i\kappa) \end{bmatrix},$$

where $\mathfrak{C}_{\pm\pm}(k, i\kappa)$ act in $\mathcal{K}_\pm$ and $\mathfrak{C}_{\mp\pm}(k, i\kappa)$ are maps of $\mathcal{K}_\mp$ to $\mathcal{K}_\pm$. The poles of $\mathfrak{C}(k, \pm ik)$, counted with multiplicities, are only finitely many, because $\det(A + BI_{n,m}(k, \pm ik))$ is a polynomial of degree not greater than $n + m$ and therefore it can have $n + m$ zeros at the most.

EXAMPLE 4.23. *Consider the operator $T(A,B)$ from Example 4.7. Then one obtains the local coefficient matrix*

$$\mathfrak{C}(k,i\kappa) = \frac{1}{\kappa^2+k^2}\begin{bmatrix} k^2-\kappa^2+2i\kappa k & 2\kappa^2-2i\kappa k \\ 2k^2+2i\kappa k & k^2-\kappa^2-2i\kappa k \end{bmatrix}.$$

The local coefficient matrix $\mathfrak{C}=\mathfrak{C}(k,ik)$ is the k–independent matrix

$$\mathfrak{C} = \begin{bmatrix} i & (1-i) \\ (1+i) & -i \end{bmatrix}.$$

This gives the generalized eigenfunction for positive energy $k>0$

$$\varphi_1(x,k,ik) = \begin{cases} e^{-ikx}+ie^{ikx}, & x\in\mathcal{E}_+, \\ (1+i)e^{-kx}, & x\in\mathcal{E}_-. \end{cases}$$

Looking at the generalized eigenfunction for positive energy $\varphi_1(\cdot,k,ik)$ one can interpret the off–diagonal entry $\mathfrak{C}_{+-}$ of $\mathfrak{C}$ as depth of penetration of the incoming wave propagating from the positive edge into the negative part of the graph. The diagonal entry $\mathfrak{C}_{++}$ describes the scattering behaviour of the incoming waves, in this example it is the reflection coefficient. The entries $\mathfrak{C}_{-+}$ and $\mathfrak{C}_{--}$ have corresponding interpretations for negative energies.

There are some useful symmetries of $\mathfrak{C}(k,i\kappa)$ summarized in the following

LEMMA 4.24. *For complex $k,\kappa\neq 0$ and A,B satisfying the assumptions of Theorem 4.2 one has*

(1) $\mathfrak{C}(k,i\kappa)^{-1}=\mathfrak{C}(-k,-i\kappa)$ *and*
(2) $\mathfrak{C}(k,ik)\begin{bmatrix}\mathbb{1} & 0\\ 0 & i\end{bmatrix} = \begin{bmatrix}\mathbb{1} & 0\\ 0 & i\end{bmatrix}\mathfrak{C}(-\overline{k},i\overline{k})^*$.
(3) *Let be $\hat{A}=P$ and $\hat{B}=P^\perp J_{n,m}$, where P is an orthogonal projector in $\mathcal{K}$. Then the matrices $\mathfrak{C}(k,ik)$ and $\mathfrak{C}(k,-ik)$ are k–independent.*

PROOF. (i) The first statement follows immediately from the definition since
$I_{n,m}(-k,-i\kappa)=-I_{n,m}(k,i\kappa)$ holds.

(ii) To prove the second statement, consider instead of A and B the equivalent parametrization given in Corollary 4.5 with

$$\hat{A}=L+P \quad\text{and}\quad \hat{B}=P^\perp\begin{bmatrix}\mathbb{1} & 0\\ 0 & -\mathbb{1}\end{bmatrix},$$

where P is an orthogonal projector and L is a Hermitian operator acting in the space $\operatorname{Ker}P$. This gives

$$\begin{aligned}&\left(\hat{A}-ikP^\perp\begin{bmatrix}\mathbb{1} & 0\\ 0 & -i\end{bmatrix}\right)\begin{bmatrix}\mathbb{1} & 0\\ 0 & i\end{bmatrix}\left(\hat{A}+ik\begin{bmatrix}\mathbb{1} & 0\\ 0 & -i\end{bmatrix}P^\perp\right)\\ &=\left(\hat{A}+ikP^\perp\begin{bmatrix}\mathbb{1} & 0\\ 0 & -i\end{bmatrix}\right)\begin{bmatrix}\mathbb{1} & 0\\ 0 & i\end{bmatrix}\left(\hat{A}-ik\begin{bmatrix}\mathbb{1} & 0\\ 0 & -i\end{bmatrix}P^\perp\right).\end{aligned}$$

For

$$\mathfrak{C}(k,ik)=\left(\hat{A}+ikP^\perp\begin{bmatrix}\mathbb{1} & 0\\ 0 & -i\end{bmatrix}\right)^{-1}\left(\hat{A}-ikP^\perp\begin{bmatrix}\mathbb{1} & 0\\ 0 & -i\end{bmatrix}\right)$$

and

$$\mathfrak{C}(\overline{k},-i\overline{k})^* = \left(\hat{A} + ik \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -i \end{bmatrix} P^\perp \right) \left(\hat{A} - ik \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -i \end{bmatrix} P^\perp \right)^{-1}$$

one obtains

$$\mathfrak{C}(k,ik) \begin{bmatrix} \mathbb{1} & 0 \\ 0 & i \end{bmatrix} \mathfrak{C}(\overline{k},-i\overline{k})^* = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & i \end{bmatrix}$$

and therefore using Part (i) of Lemma 4.24 proves the claim.

(iii) For the proof of the third part of the lemma decompose

$$P \pm ikP^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -i \end{bmatrix}$$

with respect to the orthogonal spaces Ran$P$ and Ran$P^\perp$. Denote by

$$\left(P^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mp i \end{bmatrix} P^\perp \right)^{-1} \quad \text{the inverses of} \quad P^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mp i \end{bmatrix} P^\perp$$

considered as a map in the Hilbert space Ran$P^\perp$. Applying the formula for the Schur complement, see for example [98, Theorem 1.2], delivers the k–independent block operator matrix representation

$$\mathfrak{C}(k,\pm ik) = -\left[P + ikP^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mp i \end{bmatrix}\right]^{-1} \left[P - ikP^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mp i \end{bmatrix}\right] =$$

$$\begin{bmatrix} -\left(P^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mp i \end{bmatrix} P^\perp \right)^{-1} & -\left(P^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mp i \end{bmatrix} P^\perp \right)^{-1} P^\perp \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -i \end{bmatrix} P \\ 0 & P \end{bmatrix}.$$

□

4.4.6. Resonance equation. The resonance equation (58) can be rewritten in an analogous way to the one known for Laplacians on finite metric graphs, see for example [63, Theorem 3.2]. For $k,\kappa \neq 0$ such that $(A + BI_{n,m}(k,i\kappa))$ is invertible the operator $Z_{n,m}(A,B,k,i\kappa,\underline{a})$ can be rewritten as follows

$$\begin{aligned} & Z_{n,m}(A,B,k,i\kappa,\underline{a}) \\ =& AX_{n,m}(k,i\kappa) + BY_{n,m}(k,i\kappa) \\ =& \left(A + BI_{n,m}(k,i\kappa)\right) R^+_{n,m}(k,i\kappa) + \left(A - BI_{n,m}(k,i\kappa)\right) R^-_{n,m}(k,i\kappa) \\ =& \left(A + BI_{n,m}(k,i\kappa)\right) \left(\mathbb{1} - \mathfrak{C}(k,i\kappa) T_{n,m}(k,i\kappa)\right), \end{aligned}$$

where

$$\begin{aligned} R^+_{n,m}(k,i\kappa) &= \frac{1}{2}\left(X_{n,m}(k,i\kappa) + Y_{n,m}(k,i\kappa)\right), \\ R^-_{n,m}(k,i\kappa) &= \frac{1}{2}\left(X_{n,m}(k,i\kappa) - Y_{n,m}(k,i\kappa)\right) \end{aligned}$$

becomes more explicit

$$R^{+}_{n,m}(k,i\kappa,\underline{a}) = \begin{bmatrix} R^{+}_{n}(\underline{a}_{+},k) & 0 \\ 0 & R^{+}_{m}(\underline{a}_{-},i\kappa) \end{bmatrix}, \qquad R^{+}_{l}(\underline{b},k) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & 0 & e^{ik\underline{b}} \end{bmatrix},$$

$$R^{-}_{n,m}(k,i\kappa,\underline{a}) = \begin{bmatrix} R^{-}_{n}(\underline{a}_{+},k) & 0 \\ 0 & R^{-}_{m}(\underline{a}_{-},i\kappa) \end{bmatrix}, \qquad R^{-}_{l}(\underline{b},k) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathbb{1} \\ 0 & e^{ik\underline{b}} & 0 \end{bmatrix}$$

and

$$\begin{aligned} T_{n,m}(k,i\kappa,\underline{a}) =& R^{-}_{n,m}(k,i\kappa)\left(R^{+}_{n,m}(k,i\kappa)\right)^{-1} \\ =& \begin{bmatrix} T_{n}(\underline{a}_{+},k) & 0 \\ 0 & T_{m}(\underline{a}_{-},i\kappa) \end{bmatrix}, \qquad T_{l}(\underline{b},k) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & e^{ik\underline{b}} \\ 0 & e^{ik\underline{b}} & 0 \end{bmatrix}. \end{aligned}$$

Here for $l = n$ one plugs in $\underline{b} = \underline{a}_{+}$ and for $l = m$ one inserts $\underline{b} = \underline{a}_{-}$. Assuming that $k \neq 0$ and that $A + BI_{n,m}(k, \pm ik)$ are invertible one obtains the representations

$$Z_{n,m}(A,B,k,\pm ik,\underline{a}) = (A + BI_{n,m}(k,\pm ik))\,(\mathbb{1} - \mathfrak{C}(k,\pm ik)T_{n,m}(k,\pm ik,\underline{a}))\,. \tag{62}$$

4.4.7. The resolvent. The Green's function for the equation $\left(-\frac{d^2}{dx^2} - k^2\right)u = f$ for $f \in L^2(\mathbb{R};\mathbb{C})$, is $\frac{i}{2k}e^{ik|x-y|}$. For computing the Green's function for the problem considered here, one has to find appropriate correction terms. These corrections can be expressed in terms of the solutions of the homogeneous problem $\left(\mp\frac{d^2}{dx^2} - k^2\right)u = 0$ on each edge. The Green's function obtained in this way defines an integral operator, which for $k^2 \in \mathbb{C}\setminus\mathbb{R}$ is the resolvent operator $(T(A,B) - k^2)^{-1}$. For the computation of the resolvent one follows the guide lines of [63, Section 4]. The notion of integral operators is specified in the following definition borrowed from there.

DEFINITION 4.25 ([63, Definition 4.1]). *The operator $\mathfrak{K}$ on the Hilbertspace $\mathcal{H}$ is called integral operator if for all $j, j' \in \mathcal{E}\cup\mathcal{I}$ there are measurable functions $\mathfrak{K}_{j,j'}(\cdot,\cdot)\colon I_j \times I_{j'} \to \mathbb{C}$ with the following properties*

(1) $\mathfrak{K}_{j,j'}(x_j,\cdot)\varphi_{j'} \in L^1(I_{j'};\mathbb{C})$ for almost all $x_j \in I_j$,
(2) $\psi = \mathfrak{K}\varphi$ with

$$\psi_j(x_j) = \sum_{j'\in\mathcal{E}\cup\mathcal{I}} \int_{I_{j'}} \mathfrak{K}_{j,j'}(x_j,y_{j'})\varphi_{j'}(y_{j'})dy_{j'}.$$

The $(\mathcal{I}\cup\mathcal{E})\times(\mathcal{I}\cup\mathcal{E})$ matrix-valued function $(x,y)\mapsto\mathfrak{K}(x,y)$ with

$$[\mathfrak{K}(x,y)]_{j,j'} = \mathfrak{K}_{j,j'}(x_j,y_{j'})$$

is called the integral kernel of the operator $\mathfrak{K}$.

PROPOSITION 4.26. *Let $T(A,B)$ be self–adjoint. Then the resolvent*

$$R(k^2) = (T(A,B) - k^2)^{-1}, \quad \textit{for } k^2 \in \mathbb{C}\setminus\mathbb{R},$$

is an integral operator with kernel

$$r(x,y,k) = \begin{cases} r^0_{n,m}(x,y,k,+ik) + r^1_{n,m}(x,y,k,+ik), & k \in \mathcal{Q}, \\ r^0_{n,m}(x,y,k,-ik) + r^1_{n,m}(x,y,k,-ik), & k \in \mathcal{P}, \end{cases}$$

where the free Green's function is given by

$$r^0_{n,m}(x,y,k,i\kappa) = \begin{bmatrix} r^0_n(x,y,k) & 0 \\ 0 & -r^0_m(x,y,i\kappa) \end{bmatrix} W_{n,m}(k,i\kappa),$$

where $r^0_l(x,y,k)$*,* $l \in \{n,m\}$ *are diagonal matrices with entries*

$$\{r^0_l(x,y,k)\}_{p,q} = \delta_{p,q} e^{ik|x_q - y_q|},$$

$$W_{n,m}(k,i\kappa) = \begin{bmatrix} W_n(k) & 0 \\ 0 & W_m(i\kappa) \end{bmatrix}, \qquad W_l(k) = \frac{i}{2k}\mathbb{1}_l,\ l \in \{n,m\}.$$

The correction term is given by

$$r^1(x,y,k,i\kappa) = -\Phi_{n,m}(x,k,i\kappa) G_{n,m}(k,i\kappa,\underline{a}) \Phi_{n,m}(y,k,i\kappa)^T W_{n,m}(k,i\kappa),$$

where the subscript T *denotes the transposed matrix,*

$$G_{n,m}(k,i\kappa,\underline{a}) = \mathfrak{X}(k,i\kappa)(R^+_{n,m}(k,i\kappa,\underline{a}))^{-1} J_{n,m}$$

and

$$\Phi_{n,m}(x,k,i\kappa) = \begin{bmatrix} \Phi_n(x,k) & 0 \\ 0 & \Phi_m(x,i\kappa) \end{bmatrix}$$

with

$$\Phi_l(x,k) = \begin{bmatrix} \varphi_{\mathcal{E}_l}(x,k) & 0 & 0 \\ 0 & \varphi_{\mathcal{I}_l}(x,k) & \varphi_{\mathcal{I}_l}(x,-k) \end{bmatrix}.$$

This notation means that for $l = n$ *one plugs in* $\mathcal{E}_n = \mathcal{E}_+$ *and* $\mathcal{I}_n = \mathcal{I}_+$ *and for* $l = m$ *one inserts* $\mathcal{E}_m = \mathcal{E}_-$ *and* $\mathcal{I}_m = \mathcal{I}_-$*. The blocks* $\varphi_{\mathcal{C}}(x,k)$*,* $\mathcal{C} \in \{\mathcal{E}_+, \mathcal{E}_-, \mathcal{I}_+, \mathcal{I}_-\}$ *are diagonal matrices with entries* $\{\varphi_{\mathcal{C}}(x,k)\}_{l,j\in\mathcal{C}} = \delta_{l,j}\{e^{ikx_j}\}$*.*

The proof is postponed to Appendix A. From the explicit formula in Proposition 4.26 one reads that the resolvent kernel can be defined for all $k \in \overline{\mathcal{Q}}$ as the limit of values taken from $\mathcal{Q}$, except for those $k \in \partial\mathcal{Q}$ for which $\det Z_{n,m}(A,B,k,ik,\underline{a}) = 0$. These exceptional values are called *resonances of* $T(A,B)$ *in* $\overline{\mathcal{Q}}$. Analogous for all $k \in \overline{\mathcal{P}}$ the resolvent kernel is defined, as the limit of values taken from $\mathcal{P}$, except for those $k \in \partial\mathcal{P}$ for which $\det Z_{n,m}(A,B,k,-ik,\underline{a}) = 0$. These are called the *resonances of* $T(A,B)$ *in* $\overline{\mathcal{P}}$. This justifies to denote the equations

$$\det Z_{n,m}(A,B,k,\pm ik,\underline{a}) = 0$$

the *resonance equations* for the operator $T(A,B)$.

REMARK 4.27. *From the integrability properties of the integral kernel one reads that the resolvent, as a function in* $k \in \mathcal{Q}$ *or* $k \in \mathcal{P}$*, admits a meromorphic continuation to* $\overline{\mathcal{Q}}$ *or* $\overline{\mathcal{P}}$*. The continuation is possible outside the resonances of* $T(A,B)$ *in* $\overline{\mathcal{Q}}$ *and outside the resonances of* $T(A,B)$ *in* $\overline{\mathcal{P}}$*. There the resolvent kernel* $r(\cdot,\cdot,k)$ *defines an operator*

$$R_\varepsilon(k^2)\colon L^2(\mathcal{G}, e^{\varepsilon x}dx) \to L^2(\mathcal{G}, e^{-\varepsilon x}dx), \quad \textit{for any } \varepsilon > 0.$$

Consequently outside the resonances of $T(A, B)$ *the resolvent kernel defines an operator from* $L^2_{comp}(\mathcal{G}, dx) \to L^2_{loc}(\mathcal{G}, dx)$, *where* $L^2_{comp}(\mathcal{G}, dx)$ *denotes the set of compactly supported elements of* $\mathcal{H}$ *and* L^2_{loc} *denotes the locally square integrable functions on* $(\mathcal{G}, \underline{a})$.

REMARK 4.28. *The values* k *and* $i\kappa$, *are square roots of the spectral parameters* $\lambda = k^2$ *and* $\lambda = -\kappa^2$, *respectively. In the explicit formulae involving* k *and* $i\kappa$ *it is hidden that two different branches of the complex square root are used simultaneously. To be specific, one uses the branch with* $\operatorname{Im}\sqrt{\cdot} > 0$ *and the one with* $\operatorname{Re}\sqrt{\cdot} > 0$, *respectively.*

4.5. Scattering

On the one hand, scattering theory gives an interpretation of scattering solutions in the context of time–dependent dynamics. On the other hand it gives a description of the absolutely continuous part of an operator in terms of perturbation theory. As general references for mathematical scattering theory I would like to recommend the books [11] and [96].

Here the role of the free operator is played by $T(0, \mathbb{1})$. This means that in the free system all edges are decoupled and on each positive edge one has the positive Neumann Laplace operator along with the Neumann Laplace operator multiplied by minus one on each negative edge. So, for the self–adjoint operator $T(A, B)$ one considers the scattering pair

$$(T(A, B), T(0, \mathbb{1})).$$

The pre–wave operators $W(t) \equiv W(t)\,(T(A, B), T(0, \mathbb{1}))$, where $t \in \mathbb{R}$ are defined by

$$W(t)\,(T(A, B), T(0, \mathbb{1})) := e^{itT(A,B)} e^{-itT(0,\mathbb{1})}.$$

The strong wave operators $W_\pm \equiv W_\pm\,(T(A, B), T(0, \mathbb{1}))$ are the strong limits

$$W_\pm\,(T(A, B), T(0, \mathbb{1})) := s - \lim_{t\to\pm\infty} W(t) P^{ac}_{T(0,\mathbb{1})},$$

where $P^{ac}_{T(0,\mathbb{1})}$ is the orthogonal projector onto the absolutely continuous part of $T(0, \mathbb{1})$.

THEOREM 4.29. *Let* $T(A, B)$ *be self–adjoint. Then the strong wave operators* $W_\pm$ *exist and are complete. The absolutely continuous spectrum of* $T(A, B)$ *is*

$$\sigma_{ac}(T(A, B)) = \begin{cases} (-\infty, \infty), & \text{if } \mathcal{E}_+ \neq \emptyset \text{ and } \mathcal{E}_- \neq \emptyset, \\ [0, \infty), & \text{if } \mathcal{E}_- = \emptyset \text{ and } \mathcal{E}_+ \neq \emptyset, \\ (-\infty, 0], & \text{if } \mathcal{E}_+ = \emptyset \text{ and } \mathcal{E}_- \neq \emptyset, \\ \emptyset, & \text{if } \mathcal{E}_+ = \emptyset \text{ and } \mathcal{E}_- = \emptyset. \end{cases}$$

The multiplicity of $(-\infty, 0)$ *is* $|\mathcal{E}_-|$ *and the multiplicity of* $(0, \infty)$ *is* $|\mathcal{E}_+|$.

PROOF. By Proposition 4.26 the operator

$$(T(A, B) - i)^{-1} - (T(0, \mathbb{1}) - i)^{-1}$$

is a finite rank operator and from [96, Theorem 6.5.1] it follows that the strong wave operators exist and are complete. □

4.5.1. Wave operators. In stationary scattering theory the wave operators are calculated in terms of the resolvents of the perturbed operator $T(A,B)$ and of the free operator $T(0,\mathbb{1})$. The abelian wave operators $W^a_\pm = W^a_\pm(T(A,B),T(0,\mathbb{1}))$ can be computed as

$$W^a_\pm f = \lim_{\varepsilon\to 0+} -i\varepsilon \int_{-\infty}^{\infty} R(\lambda \mp i\varepsilon) dE_0(\lambda) f,$$

where $dE_0(\cdot)$ is the absolutely continuous part of the spectral measure of the free operator and $R(\lambda\mp i\varepsilon) = (T(A,B) - (\lambda \mp i\varepsilon))^{-1}$, see [11, Proposition 13.1.1, formula (3)]. Since the strong wave operators exist they agree with the abelian wave operators, compare for example [96]. Note that the absolutely continuous part of the free operator $T(0,\mathbb{1})$ is related only to the external edges, and it can be expressed in terms of the cos-transform, see for example [93, Example 14.8]. Therefore, the absolutely continuous part of the spectral measure of the free operator $T(0,\mathbb{1})$ is

$$dE_0(\lambda) = \bigoplus_{j\in\mathcal{E}} (dE_{0,j}(\lambda)).$$

For $j\in\mathcal{E}_+$ and $\lambda>0$ one has

$$(dE_{0,j}(\lambda)f)(x) = \cos(\sqrt{\lambda}x_j)\frac{d\lambda}{\pi\sqrt{\lambda}}\int_0^\infty \cos(\sqrt{\lambda}y_j) f(y_j) dy_j,$$

and for $j\in\mathcal{E}_-$ and $\lambda<0$

$$(dE_{0,j}(\lambda)f)(x) = \cos(\sqrt{|\lambda|}x_j)\frac{d\lambda}{\pi\sqrt{|\lambda|}}\int_0^\infty \cos(\sqrt{|\lambda|}y_j) f(y_j) dy_j.$$

For the cases $j\in\mathcal{E}_+$ and $\lambda<0$, and $j\in\mathcal{E}_-$ and $\lambda>0$ one has $(dE_{0,j}(\lambda)f)(x) = 0$. Now substitute $\lambda>0$ by $k^2=\lambda$ with $k>0$ and $\lambda<0$ by $-\kappa^2=\lambda$ with $\kappa>0$. Then define on each exterior edge $j\in\mathcal{E}$ the cos-transform by

$$\hat{f}_j(k) = \frac{2}{\pi}\int_0^\infty \cos(ky_j) f(y_j) dy_j$$

and its inverse by

$$f_j(k) = \int_0^\infty \cos(ky_j)\hat{f}(k) dk.$$

Set for brevity

$$\hat{f}_+(k) = \left\{\hat{f}_j(k)\right\}_{j\in\mathcal{E}_+}, \qquad \hat{f}_-(\kappa) = \left\{\hat{f}_j(\kappa)\right\}_{j\in\mathcal{E}_-}$$

and

$$\hat{f}(k,\kappa) = \begin{bmatrix} \hat{f}_+(k) \\ \hat{f}_-(\kappa) \end{bmatrix}.$$

In the calculation of $W^a_\pm$ one can interchange the limit $\varepsilon\to 0+$ and the integration over $dE_0(\lambda)$ according to [96, Theorem 4.2.4]. After the substitution $k^2=\lambda>0$ one calculates using [96, Definition 2.7.2]

$$\lim_{\epsilon\to 0+} -i\epsilon R(k^2\pm i\epsilon) dE_0(k^2) f = \lim_{\epsilon\to 0+} -i\epsilon \int_{\mathcal{G}} r(x,y,\sqrt{k^2\pm i\epsilon}) \begin{bmatrix} \cos(kx)\hat{f}_+(k) \\ 0 \end{bmatrix} dy\, dk$$

with

$$\left\{\cos(kx)\hat{f}_+(k)\right\}_{j\in\mathcal{E}_+} = \cos(kx_j)\hat{f}_j(k)_{j\in\mathcal{E}_+}$$

and 0 denotes the zero on the rest of the components. Analogous, after substituting $-\kappa^2 = \lambda < 0$ one computes

$$\lim_{\epsilon\to 0+} -i\epsilon R(-\kappa^2 \pm i\epsilon)dE_0(-\kappa^2)f = \lim_{\epsilon\to 0+} -i\epsilon \int_{\mathcal{G}} r(x,y,\sqrt{-\kappa^2 \pm i\epsilon}) \begin{bmatrix} 0 \\ \cos(\kappa x)\hat{f}_-(\kappa) \end{bmatrix} dy\, d\kappa$$

with

$$\left\{\cos(\kappa x)\hat{f}_-(\kappa)\right\}_{j\in\mathcal{E}_-} = \cos(\kappa x_j)\hat{f}_j(\kappa)_{j\in\mathcal{E}_-}$$

and again 0 denotes the zero on the rest of the components. This calculation is carried out in Appendix B. The result is that the strong wave operators can be computed in terms of the generalized eigenfunctions of $T(A,B)$.

PROPOSITION 4.30. *For $f \in \operatorname{Ran} P^{ac}_{T(0,\mathbb{1})} = \mathcal{H}_{\mathcal{E}}$ one has*

$$W_+ f = \sum_{l\in E_+} \int_0^\infty \varphi_l(\cdot, -k, ik)\hat{f}_l(k)\tfrac{dk}{2} + \sum_{l\in E_-} \int_0^\infty \varphi_l(\cdot, ik, k)\hat{f}_l(k)\tfrac{dk}{2}$$

and

$$W_- f = \sum_{l\in E_+} \int_0^\infty \varphi_l(\cdot, k, ik)\hat{f}_l(k)\tfrac{dk}{2} + \sum_{l\in E_-} \int_0^\infty \varphi_l(\cdot, ik, -k)\hat{f}_l(k)\tfrac{dk}{2}.$$

REMARK 4.31. *From Theorem 4.29 it follows that the absolutely continuous part of $T(A,B)$ is the range of $W_\pm$. Hence, spectral representations of the absolutely continuous part of $T(A,B)$ are given by the transforms*

$$U_\pm = W_\pm W_\pm^*.$$

4.5.2. Scattering matrix. As the wave operators exist and since they are complete one can define the scattering operator $S \equiv S\left(T(A,B), T(0,\mathbb{1})\right)$ by

$$S := W_+^* W_-.$$

The scattering operator is a unitary operator on the absolutely continuous subspace of $T(0,\mathbb{1})$. From the formulae for the wave operators given in Proposition 4.30 one sees that the wave operators decompose into two parts. One part is related to the positive absolutely continuous spectrum and the other part is related to the negative absolutely continuous spectrum. This observation can be formalized within the concept of local wave operators, see for example [96, Chapter 2.2.2]. The local wave operators $W_\pm(\Lambda) \equiv W_\pm(T(A,B), T(0,\mathbb{1}), \Lambda)$ are

$$W_\pm\left(T(A,B), T(0,\mathbb{1}), \Lambda\right) := s - \lim_{t\to\pm\infty} e^{itT(A,B)}e^{-itT(0,\mathbb{1})}P_0^{ac}(\Lambda),$$

where $\Lambda \subset \sigma_{ac}(T(0,\mathbb{1}))$ and $P_0^{ac}(\cdot)$ is the spectral projector of the absolutely continuous part of the free operator $T(0,\mathbb{1})$. For $\Lambda_+ = [0,\infty)$ and $\Lambda_- = (-\infty, 0]$ one has furthermore, because $|\Lambda_+ \cap \Lambda_-| = 0$, that

$$W_\pm = W_\pm(\Lambda_+) + W_\pm(\Lambda_-).$$

The local wave operators $W_{\pm}\left(\Lambda_{+}\right)$ are

$$W_{+}\left(\Lambda_{+})\right) f = \sum_{l\in E_{+}} \int_0^\infty \varphi_l(\cdot,-k,ik)\hat{f}_l(k)\tfrac{dk}{2},$$

$$W_{+}\left(\Lambda_{-})\right) f = \sum_{l\in E_{-}} \int_0^\infty \varphi_l(\cdot,ik,k)\hat{f}_l(k)\tfrac{dk}{2}$$

and

$$W_{-}\left(\Lambda_{+}\right) f = \sum_{l\in E_{+}} \int_0^\infty \varphi_l(\cdot,k,ik)\hat{f}_l(k)\tfrac{dk}{2},$$

$$W_{-}\left(\Lambda_{-}\right) f = \sum_{l\in E_{-}} \int_0^\infty \varphi_l(\cdot,ik,-k)\hat{f}_l(k)\tfrac{dk}{2}.$$

For the scattering operator it follows that

$$S = W_{+}\left(\Lambda_{+}\right)^{*} W_{-}\left(\Lambda_{+}\right) + W_{+}\left(\Lambda_{-}\right)^{*} W_{-}\left(\Lambda_{-}\right).$$

Let U^0 be a given spectral representation for the free operator, then the corresponding *scattering matrix* for U_0 is defined as

$$S(\cdot) = U_0 W_+^* W_- U_0^*.$$

The scattering matrix is unitary. Here one chooses U_0 to be the diagonal block-operator matrix

$$U_0 = \begin{bmatrix} U_0^+ & 0 \\ 0 & U_0^- \end{bmatrix}, \quad \text{where} \quad U_0^+ f = \hat{f}_+, \text{ and } U_0^- f = \hat{f}_-.$$

This is the cos-transform for the absolutely continuous part of the free operator $T(0,\mathbb{1})$, that already appeared in the context of stationary scattering theory. As a consequence the scattering matrix is a diagonal block operator matrix. Using Proposition 4.30 the scattering matrix can be computed in terms of the coefficients of the generalized eigenfunctions. In the following this is carried out in detail.

Write $\varphi_l(\pm k, i\kappa, x)$, where $l\in\mathcal{E}$, into the $|\mathcal{E}|\times|\mathcal{E}\cup\mathcal{I}|$–matrix $\Phi(x,\pm k,ik)$ with entries

$$\left\{\Phi(x,\pm k,ik)\right\}_{j,l} := \left\{\varphi_l(x,\pm k,i\kappa)\right\}_j.$$

The restrictions of $\Phi(x,\pm k,ik)$ to $\mathcal{E}_+$ are

$$\left\{\Phi(x,+k,ik)\right\}_{j,l\in\mathcal{E}_+} = \delta_{lj}e^{-ikx_j} + e^{ikx_l}\chi_{j,l}(k,ik)$$

and

$$\left\{\Phi(x,-k,ik)\right\}_{j,l\in\mathcal{E}_+} = \delta_{lj}e^{ikx_j} + e^{-ikx_l}\chi_{j,l}(-k,ik).$$

Consider the restriction of $\chi(k,ik)$ to the external edges and denote it by $\chi_{\mathcal{E},\mathcal{E}}(k,i\kappa)$, which is a $|\mathcal{E}|\times|\mathcal{E}|$–matrix with entries

$$\{\chi(k,i\kappa)_{\mathcal{E},\mathcal{E}}\}_{j,l\in\mathcal{E}} = \left\{\chi(k,i\kappa)\right\}_{j,l\in\mathcal{E}}.$$

With respect to the division into positive and negative external edges one obtains the block structure

$$\chi_{\mathcal{E},\mathcal{E}}(k,i\kappa) = \begin{bmatrix} \chi_{++}(k,i\kappa) & \chi_{+-}(k,i\kappa) \\ \chi_{-+}(k,i\kappa) & \chi_{--}(k,i\kappa) \end{bmatrix}, \tag{63}$$

where $\chi_{p,q}(k,i\kappa)$ with $p,q\in\{+,-\}$ are the matrices with entries

$$\{\chi(k,i\kappa)_{p,q}\}_{j\in\mathcal{E}_p,l\in\mathcal{E}_q}=\{\chi(k,i\kappa)\}_{j\in\mathcal{E}_p,l\in\mathcal{E}_q}.$$

Since the functions e^{-ikx} and e^{ikx} are on each edge linearly independent there exists a $|\mathcal{E}_+|\times|\mathcal{E}_+|$–matrix $C_+(k)$ with entries $\{C_+(k)\}_{l,j\in\mathcal{E}_+}=c_{lj}(k)$ such that

$$\Phi(\cdot,k,ik)C_+(k)=\Phi(\cdot,-k,ik)$$

holds on the positive external edges. The functions $c_{lj}(k)\varphi_l(\cdot,k,ik)$ are generalized eigenfunctions as well and therefore their linear combinations

$$\varphi_j(\cdot,-k,ik)=\sum_{l\in\mathcal{E}_+}c(k)_{lj}\varphi_l(\cdot,k,ik),\quad\text{for } x\in\mathcal{E}_+$$

are generalized eigenfunctions, too. Recall that the functions $\varphi_l(\cdot,k,ik)$ and $\varphi_l(\cdot,-k,ik)$ are defined uniquely up to a set of measure zero. Hence the relation

$$\varphi_j(\cdot,-k,ik)=\sum_{l\in\mathcal{E}_+}c(k)_{lj}\varphi_l(\cdot,k,ik)$$

carries over from the external parts to the whole graph $(\mathcal{G},\underline{a})$. Comparing the coefficients on the external edges yields

$$C_+(k)\chi_{++}(k,ik)=\mathbb{1}_{\mathcal{E}_+}\quad\text{and hence}\quad C_+(k)^{-1}=\chi_{++}(k,ik).$$

Analogously one obtains

$$\varphi_l(\cdot,ik,k)=\sum_{l\in\mathcal{E}_-}c_{lj}(k)\varphi_l(\cdot,ik,-k),$$

for an appropriate $|\mathcal{E}_-|\times|\mathcal{E}_-|$–matrix $C_-(k)$ with entries $\{C_-(k)\}_{j,l\in\mathcal{E}_-}=c_{lj}(k)$. Considering the restriction of $\varphi_l(\cdot,ik,\pm k)$ to $\mathcal{E}_-$ yields

$$\Phi(\cdot,ik,-k)C_-(k)=\Phi(\cdot,ik,k)$$

and hence

$$C_-(k)\chi_{--}(ik,k)=\mathbb{1}_{\mathcal{E}_-}\quad\text{and}\quad C_-(k)^{-1}=\chi_{--}(ik,k).$$

This can be used to express W_- in terms of W_+ as follows,

$$W_+M_CU_0f=W_-f,\tag{64}$$

where M_C denoted the multiplication operator with $C(\cdot)$,

$$C(k)=\begin{bmatrix}C_+(k)&0\\0&C_-(k)\end{bmatrix}\quad\text{and hence } M_C\hat{f}_\pm(k)=C_\pm(k)\hat{f}_\pm(k).$$

As the absolutely continuous parts of $T(\mathbb{1},0)$ and $T(A,B)$ are unitarily equivalent one can introduce the wave matrices using for example the transform U_- from Remark 4.31. Here the wave matrices w_+ and w_- are defined by

$$w_+(k)\hat{f}(k)=U_-W_+U_0^*\hat{f}(k)\quad\text{and}\quad w_-(k)\hat{f}(k)=U_-W_-U_0^*\hat{f}(k),$$

and they are unitary maps from $\operatorname{Ran}U_0$ to Ran U_-. With the above equation (64) one obtains using $U_0^*U_0f=U_0^*\hat{f}$ that

$$w_+^*w_-\hat{f}_+=M_{C_+}^*\hat{f}_+\quad\text{and}\quad w_+^*w_-\hat{f}_-=M_{C_-}^*\hat{f}_-,$$

where $M^*_{C_\pm}$ are the multiplication operators with $C^*_\pm(\cdot)$. By the definitions of w_+ and w_- one has for the scattering matrix

$$S(k^2)\hat{f}(k) = w_+^*(k)w_-(k)\hat{f}(k)$$

and hence $C_+(k)$ is unitary for almost all $k > 0$ and as $C_+(k)^{-1} = \chi_{++}(k, ik)$ one concludes that $C_+(k)^* = \chi_{++}(k, ik)$. Analogously one obtains $C_-(k)^* = \chi_{--}(ik, k)$. This is summarized in

THEOREM 4.32. *Let $T(A,B)$ be self–adjoint. Then the scattering matrix for the pair $(T(A,B), T(0,\mathbb{1}))$ is a $|\mathcal{E}_+| \times |\mathcal{E}_+|$–matrix for positive energies $\lambda > 0$ and a $|\mathcal{E}_-| \times |\mathcal{E}_-|$–matrix for negative energies $\lambda < 0$,*

$$S(\lambda) = \begin{cases} \chi_{++}(\sqrt{\lambda}, i\sqrt{\lambda}), & \lambda > 0, \\ \chi_{--}(i\sqrt{|\lambda|}, \sqrt{|\lambda|}), & \lambda < 0, \end{cases}$$

where χ_{++} and χ_{--} have been defined in equation (63) *as restrictions of the coefficient χ.*

Recall that the coefficient χ has been defined in (60). Especially one obtains, applying Theorem 4.32 to star–graphs, the non–obvious fact that the blocks $\mathfrak{C}_{++}(k, ik)$ and $\mathfrak{C}_{--}(ik, k)$ of the coefficient matrix $\mathfrak{C}(k, ik)$ defined in equation (61), are unitary for all $k > 0$, except a finite set. The relevance of Theorem 4.32 arises from the fact that it justifies to read the scattering properties of the system directly from the coefficients of the generalized eigenfunctions. This is common when considering self–adjoint Laplacians on graphs, but it is not self–evident, as shown for the example of a Schrödinger operator on the real line with step potential. In this case one obtains a relation between the coefficients of the generalized eigenfunctions and the scattering matrix as well, but both do not agree in general, compare for example [44]. Overall, the articles [44, 45] have been useful for the understanding of the scattering problem considered here.

EXAMPLE 4.33. *Consider the graph that consists of two external edges $\mathcal{E}_+ = \{1, 2\}$ which are connected by an internal edge $I_- = \{3\}$ of length $\underline{a} = \{a\}$. This means that one has the two vertices $\partial(1) = \partial_-(3)$ and $\partial(2) = \partial_+(3)$. The boundary conditions imposed on each vertex are the standard boundary conditions from Example 4.7. They are encoded in the matrices*

$$A = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \textit{and} \quad B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{bmatrix}.$$

Hence one obtains

$$X_{2,2}(k, ik, \underline{a}) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & e^{-ka} & e^{ka} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, Y_{2,2}(k, ik, \underline{a}) = \begin{bmatrix} ik & 0 & 0 & 0 \\ 0 & -k & +k & 0 \\ 0 & ke^{-ka} & -ke^{ka} & 0 \\ 0 & 0 & 0 & ik \end{bmatrix}$$

and with $Z_{2,2}(A, B, k, ik, \underline{a}) = AX_{2,2}(k, ik, \underline{a}) + BY_{2,2}(k, ik, \underline{a})$ one obtains the scattering matrix for $k > 0$

$$S(k^2) = \begin{bmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{bmatrix} = \begin{bmatrix} i\tanh(ak) & \frac{1}{\cosh(ak)} \\ \frac{1}{\cosh(ak)} & i\tanh(ak) \end{bmatrix}.$$

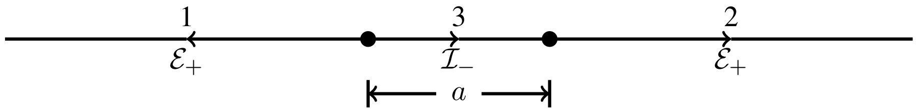


FIGURE 6. The graph described in Example 4.33.

The absolutely continuous spectrum is $[0,\infty)$ *with multiplicity two. The negative eigenvalues are the zeros of*

$$\det Z_{2,2}(A,B,ik,k,\underline{a}) = k^2\cos(ak)$$

and there are no embedded eigenvalues. Hence the pure point spectrum of $T(A,B)$

$$\sigma_{pp}(T(A,B)) = \left\{ -\left(\frac{((2m-1)\pi)^2}{2a}\right)^2 \,\middle|\, m\in\mathbb{N}\right\}$$

consists of infinitely many negative eigenvalues with multiplicity one accumulating at $-\infty$*. The kernel is zero and there are no further resonances.*

EXAMPLE 4.34. *For the situation considered in Example 4.23 one reads from Theorem 4.32 that the scattering matrix is*

$$S(\lambda) = \begin{cases} +i, & \lambda > 0,\\ -i, & \lambda < 0.\end{cases}$$

The absolutely continuous spectrum is the whole real line and there are no eigenvalues.

EXAMPLE 4.35. *Consider a star graph with three edges,* $\mathcal{E}_+ = \{1,2\}$ *and* $\mathcal{E}_- = \{3\}$ *matched together by the boundary conditions*

$$A = \begin{bmatrix} 1 & -1 & 0\\ 0 & 1 & -1\\ 0 & 0 & 0\end{bmatrix} \quad\text{and}\quad B = \begin{bmatrix} 0 & 0 & 0\\ 0 & 0 & 0\\ 1 & 1 & -1\end{bmatrix}.$$

Note that these local boundary conditions are the ones derived in Section 4.2. The operator $T(A,B)$ *has absolutely continuous spectrum* $(-\infty,\infty)$*, where* $(0,\infty)$ *has multiplicity two and* $(-\infty,0)$ *has multiplicity one. Since*

$$\det Z_{2,1}(A,B,k,i\kappa) = \kappa + 2ik,$$

there are no eigenvalues and no resonances. The local coefficient matrix ,

$$\mathfrak{C}(k,ik) = \mathfrak{C} = \begin{bmatrix} -1/5+(2/5)i & 4/5+(2/5)i & 2/5-(4/5)i\\ 4/5+(2/5)i & -1/5+(2/5)i & 2/5-(4/5)i\\ 4/5+(2/5)i & 4/5+(2/5)i & -3/5-(4/5)i\end{bmatrix}$$

is k*–independent and the scattering matrix is given by the corresponding blocks of* $\mathfrak{C} = \chi_{\mathcal{E},\mathcal{E}}$*,*

$$S(\lambda) = \begin{cases} \begin{bmatrix} -1/5+(2/5)i & 4/5+(2/5)i\\ 4/5+(2/5)i & -1/5+(2/5)i\end{bmatrix}, & \lambda > 0,\\ -3/5-(4/5)i, & \lambda < 0.\end{cases}$$

Looking at the generalized eigenfunctions and taking into account Theorem 4.32 one can try an interpretation of the coefficient matrix $\mathfrak{C}(k,ik)$. Let $\mathcal{G}$ be a star graph and $k>0$, then

- $\mathfrak{C}_{++}(k, ik)$ is the scattering matrix, that is the entries describe the transmitted and reflected parts of an incoming wave (scattering matrix for positive energies),
- $\mathfrak{C}_{+-}(k, ik)$ is the depth of indentation of an incoming wave with positive energy k^2 into the negative part of the graph.

For negative energies $-k^2 < 0$ the matrices $\mathfrak{C}_{--}(ik, -k)$ and $\mathfrak{C}_{-+}(ik, -k)$ admit analogous interpretations.

4.5.3. Time–dependent Problems. A delicate topic dealing with indefinite operators is to consider time–dependent problems. Thinking of applications to solid-state physics, one considers the Schrödinger equation. In the effective mass approximation, the effective mass tensor can be negative, too. For any self–adjoint operator one can now give the solutions of the initial value problem

$$\begin{cases} \left(i\dfrac{\partial}{\partial t} - T(a,b)\right) u(x,t) = 0, \\ \\ u(\cdot, 0) = u_0, \quad \text{for } t \in \mathbb{R}. \end{cases}$$

in terms of a unitary group

$$u = U(t)u_0, \quad \text{where} \quad U(t) = e^{-itT(A,B)}$$

is acting in $\mathcal{H}$. The fact that the spectrum is not semi–bounded is no obstacle for the construction of this group, similar to the situation, when considering the Dirac equation.

Considering the wave equation or the diffusion equation changes this feature completely. The lower bound on the spectrum of a semi–bounded operator can be interpreted as a measure for the stability of the system. Problems that arise when the spectrum is neither bounded from below nor from above can be avoided by projecting away the critical parts of the spectrum. Assume that $\mathcal{E}_- = \emptyset$ and consider a self-adjoint operator $T(A, B)$ on such a graph. Then $T(A, B)$ has only positive absolutely continuous spectrum. Denote by $T_{ac}(A, B)$ the restriction of $T(A, B)$ onto its absolutely continuous subspace. For the wave equation according to [11, Chapter 10.3] with $\mathcal{B} = T_{ac}(A, B)^{1/2}$ the solution of

$$\left(\frac{\partial^2}{\partial t^2} + T_{ac}(A,B)\right) u(x,t) = 0, \qquad u(0) = u_0, \qquad \frac{\partial}{\partial t} u = v_0$$

is given by the group

$$\begin{bmatrix} u(t) \\ u'(t) \end{bmatrix} = \begin{bmatrix} \cos(\mathcal{B}t) & \mathcal{B}^{-1}\sin(t\mathcal{B}) \\ -\mathcal{B}\sin(t\mathcal{B}) & \cos(t\mathcal{B}) \end{bmatrix} \begin{bmatrix} u_0 \\ v_0 \end{bmatrix},$$

acting in an appropriate Hilbert space. All entries are known in terms of the spectral theorem using the spectral transform of $T_{ac}(A, B)$, which in turn is explicitly given in terms of generalized eigenfunctions, compare Remark 4.31 and Proposition 4.30.

Alternatively one can consider a piecewise defined wave equation

$$\begin{cases} +\left(\frac{\partial^2}{\partial t^2} - \frac{d^2}{dx^2}\right) u(x,t) = 0, \quad x \in \mathcal{G}_+, \\ \\ -\left(\frac{\partial^2}{\partial t^2} - \frac{d^2}{dx^2}\right) u(x,t) = 0, \quad x \in \mathcal{G}_- \end{cases}$$

with appropriate initial conditions. This would correspond to a completely reversed dynamics on the negative part compared to the positive one. Such problems – although very interesting – are beyond the scope of the approach presented here.

4.5.4. Gluing formula for the scattering matrix. Let be given two connected metric graphs. Then one can construct a single connected metric graph by gluing the two original graphs together along external edges. Each two external edges glued together in pairs, become an internal edge of a certain length. To be more precise, let be given two metric graphs $(\mathcal{G}_1, \underline{a}_1)$, where $\mathcal{G}_1 = (V_1, \mathcal{I}_1, \mathcal{E}_1, \partial_1)$ and $(\mathcal{G}_2, \underline{a}_2)$, where $\mathcal{G}_2 = (V_2, \mathcal{I}_2, \mathcal{E}_2, \partial_2)$. Furthermore let be given two subsets $\tilde{\mathcal{E}_1} \subset \mathcal{E}_1$ and $\tilde{\mathcal{E}_2} \subset \mathcal{E}_2$ of their external edges with $|\tilde{\mathcal{E}_1}| = |\tilde{\mathcal{E}_2}|$, and a bijective identification map

$$G\colon \tilde{\mathcal{E}_1} \to \tilde{\mathcal{E}_2}.$$

Then define a new graph

$$\mathcal{G} := \mathcal{G}_1 \circ_G \mathcal{G}_2$$

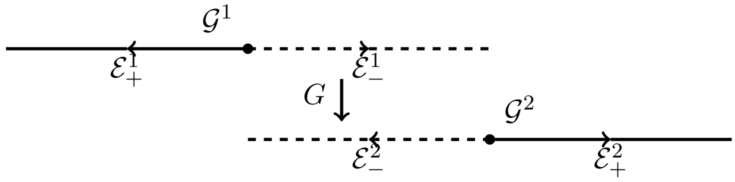
by $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ with $V = V_1 \cup V_2$ and $\mathcal{E} = \left(\mathcal{E}_1 \setminus \tilde{\mathcal{E}_1}\right) \cup \left(\mathcal{E}_2 \setminus \tilde{\mathcal{E}_2}\right)$; the internal edges are $\mathcal{I} = \mathcal{I}_1 \cup \mathcal{I}_2 \cup \mathcal{I}_G$, where $\mathcal{I}_G$ are the new edges connecting the two graphs, and one has $|\mathcal{I}_G| = |\tilde{\mathcal{E}_1}|$. Any element $e \in \tilde{\mathcal{E}_1}$ becomes an element of $i = i_e \in \mathcal{I}_G$ and one sets $\partial(i_e) = (\partial(e), \partial(G(e)))$. Assigning to each new internal length edge the length a_i, which is written into $\underline{a}_G = \{a_i\}_{i \in \mathcal{I}_G}$ and keeping the edge lengths of $\mathcal{I}_1$ and $\mathcal{I}_2$ one obtains a new metric graph $(\mathcal{G}, \underline{a})$.

Let there be furthermore two self–adjoint Laplace operators defined on each of the metric graphs $(\mathcal{G}_j, \underline{a}_j)$, $j = 1, 2$. Then their boundary conditions define naturally a self–adjoint operator on the new graph $\mathcal{G} = \mathcal{G}_1 \circ_G \mathcal{G}_2$, constructed by gluing together the two original ones. One can consider first the scattering matrices of the operators defined on each of the components separately. Then the scattering matrix of the operator defined on the new graph can be computed in terms of the original data of the scattering matrices and the data used in the gluing construction. This iterative process is known as *star product*. The history of star products for scattering matrices goes back to R. Redheffer, see [81, 82]. The star product for Laplacians on metric graphs has been studied by V. Kostrykin and R. Schrader, see [60, 61]. The considerations presented here are based on these last mentioned works. For the history of the star products and factorizations of the scattering matrix see also the references quoted therein. Such gluing formulae are only known for one dimensional (singular) spaces. For higher dimensions such formulae are not known in general.

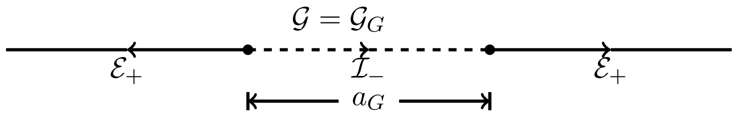
Here a gluing formula is presented for the case of two graphs which have equal numbers of negative external edges and all of them are glued together in pairs. This permits to use the generalized star product for studying scattering properties of systems where the negative part of the leading coefficient is only compactly supported.

Consider two finite metric graphs $(\mathcal{G}^1, \underline{a}^1)$ and $(\mathcal{G}^2, \underline{a}^2)$ with $|\mathcal{E}^1_-| = |\mathcal{E}^2_-|$, and on each of these graphs the self–adjoint operators $T(A_1, B_1)$ and $T(A_2, B_2)$, respectively. In addition let there be a bijective identification $G\colon \mathcal{E}^1_- \to \mathcal{E}^2_-$. One considers now the graph $\mathcal{G} = \mathcal{G}_1 \circ_G \mathcal{G}_2$ with $\mathcal{I}_G \subset \mathcal{I}_-$ and lengths $a_i > 0$ for $i \in \mathcal{I}_G$. The boundary conditions (A_1, B_1) and (A_2, B_2) act only on V_1 or on V_2, respectively. Therefore one can impose on $\mathcal{G}$ the boundary conditions defined by

$$A = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix},$$



(a) Two disconnetcted star graphs and the identification map G



(b) Connected graph after gluing construction with internal edge length a_G

FIGURE 7. Two graphs glued along the negative external edges.

which are given with respect to the division $V = V_1 \dot{\cup} V_2$. Hence $T(A, B)$ is self–adjoint on $\mathcal{G}$ for any choice of $\underline{a}_G$.

Let $\chi^j(k, ik)$ be the coefficients of the generalized eigenfunctions of $T(A_j, B_j)$ on $(\mathcal{G}^j, \underline{a}^j)$, for $j = 1, 2$. With respect to the decomposition into positive and negative external edges one writes as in equation (63)

$$\chi^1_{\mathcal{E}^1,\mathcal{E}^1}(k, ik) = \begin{bmatrix} \chi^1_{++}(k, ik) & \chi^1_{+-}(k, ik) \\ \chi^1_{-+}(k, ik) & \chi^1_{--}(k, ik) \end{bmatrix}$$

and

$$\chi^2_{\mathcal{E}^2,\mathcal{E}^2}(k, ik) = \begin{bmatrix} \chi^2_{++}(k, ik) & \chi^2_{+-}(k, ik) \\ \chi^2_{-+}(k, ik) & \chi^2_{--}(k, ik) \end{bmatrix}.$$

The operator $T(A, B)$ on the metric graph $(\mathcal{G}, \underline{a})$, obtained by gluing together both along the negative edges, with new lengths $\underline{a}_G$, has only positive absolutely continuous spectrum and its scattering matrix is explicitly computable in terms of $\chi^1_{\mathcal{E}^1,\mathcal{E}^1}(k, ik)$ and $\chi^2_{\mathcal{E}^2,\mathcal{E}^2}(k, ik)$, assuming some compatibility properties. To make these compatibility assumptions more precise one denotes the critical sets where the generalized star product is a priori not defined by

$$\begin{aligned} \Xi_1(\chi^1, \chi^2, \underline{a}) &:= \left\{ k > 0 \mid \det[\mathbb{1} - e^{-k\underline{a}} \chi^1_{--}(k, ik) e^{-k\underline{a}} \chi^2_{--}(k, ik)] = 0 \right\}, \\ \Xi_2(\chi^1, \chi^2, \underline{a}) &:= \left\{ k > 0 \mid \det[\mathbb{1} - e^{-k\underline{a}} \chi^2_{--}(k, ik) e^{-k\underline{a}} \chi^1_{--}(k, ik)] = 0 \right\} \end{aligned}$$

and by

$$\Theta(\chi^1, \chi^2) = \left\{ k > 0 \mid k \text{ singularity of } \chi^1(k, ik) \text{ or } \chi^2(k, ik) \right\}.$$

The generalized star product is defined in [61] and denoted by $*_p$. The gluing formula is described in the following

PROPOSITION 4.36. *Let $T(A_1, B_1)$ and $T(A_2, B_2)$ be self–adjoint operators on $(\mathcal{G}^1, \underline{a}^1)$ and on $(\mathcal{G}^2, \underline{a}^2)$, respectively, where $p = |\mathcal{E}^1_-| = |\mathcal{E}^2_-|$. Let furthermore be $T(A, B)$ and $(\mathcal{G}, \underline{a})$ as described above. Then for all $k > 0$ with $k \notin \Xi_1(\chi^1, \chi^2, \underline{a}) \cup \Xi_2(\chi^1, \chi^2, \underline{a}) \cup \Theta(\chi^1, \chi^2)$ the* *scattering matrix of the pair $(T(A,B), T(0,\mathbb{1}))$ is given in terms of the generalized star product as*

$$S(k^2) = \chi^1_{\mathcal{E},\mathcal{E}}(k,ik) *_p V(\underline{a}_G,k)\chi^2_{\mathcal{E},\mathcal{E}}(k,ik), \qquad V(\underline{a}_G,k) = \begin{bmatrix} e^{-k\underline{a}_G} & 0 \\ 0 & \mathbb{1} \end{bmatrix}.$$

Carrying this out gives

$$S(k^2) = \begin{bmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{bmatrix},$$

where the blocks $s_{ij}(k)$, $i,j \in \{1,2\}$ of the scattering matrix are matrices with entries

$$\{s_{ij}(k)\}_{n,m} = \{(s_{n,m}(k))\}_{n\in\mathcal{E}^i_+, m\in\mathcal{E}^j_+},$$

and one has

$$\begin{aligned}
s_{11} =& \chi^1_{++} + \chi^1_{+-} e^{-k\underline{a}_G}\chi^2_{--}e^{-k\underline{a}_G}[\mathbb{1} - \chi^1_{--}e^{-k\underline{a}_G}\chi^2_{--}e^{-k\underline{a}_G}]^{-1}\chi^1_{-+},\\
s_{21} =& \chi^2_{+-}e^{-k\underline{a}_G}[\mathbb{1} - \chi^1_{--}e^{-k\underline{a}_G}\chi^2_{--}e^{-k\underline{a}_G}]^{-1}\chi^1_{-+},\\
s_{12} =& \chi^1_{+-}[\mathbb{1} - e^{-k\underline{a}_G}\chi^2_{--}e^{-k\underline{a}_G}\chi^1_{--}e^{-k\underline{a}_G}]^{-1}e^{-k\underline{a}_G}\chi^2_{-+},\\
s_{22} =& \chi^2_{++} + \chi^2_{+-}e^{-k\underline{a}_G}\chi^1_{--}e^{-k\underline{a}_G}[\mathbb{1} - e^{-k\underline{a}_G}\chi^2_{--}e^{-k\underline{a}_G}\chi^1_{--}]^{-1}e^{-k\underline{a}_G}\chi^2_{-+},
\end{aligned}$$

where the k–dependence is omitted and $\chi^j_{\pm,\pm}$ is short for $\chi^j_{\pm,\pm}(k,ik)$, $j = 1,2$.

The proof is completely analogous to the proof given in [61], and it is therefore omitted here. It is based on the fact that the generalized eigenfunctions of the new problem can be obtained as linear combinations of the generalized eigenfunctions of the two original scattering problems. The restriction imposed on the energies for which the gluing formula is valid is due to the fact that, in contrast to the case of self–adjoint Laplacians on graphs, the relation between eigenvalues and resonances has not been clarified yet.

The formula in Proposition 4.36 shows that for positive energies the matrix $V(\underline{a},k)$ damps the scattering waves on $\mathcal{I}_G$ down. Let be $k_n > 0$ with

$$k_n \notin \Xi_1(\chi^1,\chi^2,\underline{a}) \cup \Xi_2(\chi^1,\chi^2,\underline{a}) \cup \Theta(\chi^1,\chi^2), \quad n \in \mathbb{N},$$

and $k_n \to \infty$ for $n \to \infty$ and assume that the limits

$$\lim_{n\to\infty} \chi^1_{++}(k_n) \quad \text{and} \quad \lim_{n\to\infty} \chi^2_{++}(k_n) \tag{65}$$

exist. As a direct consequence of Proposition 4.36 one obtains then

$$\lim_{n\to\infty} s_{12}(k_n) = 0, \qquad \lim_{n\to\infty} s_{21}(k_n) = 0$$

and

$$\lim_{n\to\infty} s_{11}(k_n) = \lim_{n\to\infty} \chi^1_{++}(k_n), \qquad \lim_{n\to\infty} s_{22}(k_n) = \lim_{n\to\infty} \chi^2_{++}(k_n).$$

This shows that the scattering matrix resembles for large energies the direct sum of the scattering matrices of the two building stones. However it is not clear that the limits in (65) do always exist.

REMARK 4.37. *Gluing together positive as well as negative edges can be done in two steps. First, one together glues the negative edges, and then one considers this graph and an auxiliary* *graph consisting of two edges with continuity boundary conditions. This is used to connect two positive edges. More precisely, after having constructed*

$$S(k^2) = \chi^1_{\mathcal{E},\mathcal{E}}(k, ik) *_p V(\underline{a}_G, k)\chi^2_{\mathcal{E},\mathcal{E}}(k, ik)$$

according to Proposition 4.36 one considers the auxiliary graph $\mathcal{G}_{aux} = (V, \mathcal{E}, \partial)$, $|V| = 1$, $|\mathcal{E}| = 2$ *and the Laplacian defined on it by the boundary conditions*

$$A = \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix} \quad \textit{and} \quad B = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}.$$

This operator $-\Delta_{aux} = -\Delta(A, B)$ *has the scattering matrix* $S_{aux}(k^2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. *Now one glues together two external edges of* $\mathcal{G}$ *and replaces them by an internal edge of length* a. *The scattering matrix of this new problem is*

$$S(k^2) *_2 \begin{bmatrix} e^{ika} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

This analogous to the results obtained in [61].

EXAMPLE 4.38. *Consider again Example 4.33. The graph described there can be obtained also by gluing two star graphs, where each is a copy of the graph given in Example 4.7. These are glued together along the negative edges, which gives a new negative internal edge of a certain length* $\underline{a} = \{a\}$. *The coefficient matrices* $\mathfrak{C}^j = \mathfrak{C}^j(k, ik)$ *are*

$$\mathfrak{C}^j = \begin{bmatrix} \chi^j_{++}(k, ik) & \chi^j_{+-}(k, ik) \\ \chi^j_{-+}(k, ik) & \chi^j_{--}(k, ik) \end{bmatrix} = \begin{bmatrix} i & (1-i) \\ (1+i) & -i \end{bmatrix}, \quad j = 1, 2,$$

see Example 4.23. Using the gluing formula from Proposition 4.36 with new edge length a *one obtains*

$$\begin{aligned} s_{11}(k) =& \chi^1_{++} + \chi^1_{+-}e^{-ka}\chi^2_{--}e^{-ka}[\mathbb{1} - \chi^1_{--}e^{-ka}\chi^2_{--}e^{-ka}]^{-1}\chi^1_{-+} \\ =& i\tanh(ka) \end{aligned}$$

and

$$\begin{aligned} s_{21}(k) =& \chi^2_{+-}e^{-ka}[\mathbb{1} - \chi^1_{--}e^{-ka}\chi^2_{--}e^{-ka}]^{-1}\chi^1_{-+} \\ =& \frac{1}{\cosh(ka)}. \end{aligned}$$

This is well defined for any $k > 0$. *For symmetry reasons one has* $s_{22}(k) = s_{11}(k)$ *and* $s_{21}(k) = s_{12}(k)$. *Applying the gluing formula yields the same result as the direct calculation in Example 4.33. Note that the limits*

$$\lim_{k\to 0} S(k^2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \textit{and} \quad \lim_{k\to\infty} S(k^2) = \begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix}$$

exist. For small energies there is full transmission, whereas for large energies there is full reflection along with a phase shift. In addition, the scattering matrix resembles for large energies the direct sum of the scattering matrices of the two building stones which have been discussed in Example 4.34. This is a feature not known for scattering systems involving only semi–bounded operators.

4.5.5. Scattering and cloaking phenomena? In the article [22] the light propagation through metamaterials is described using regularizations of the indefinite operator

$$\tau u = -\operatorname{div} A(\cdot) \operatorname{grad} u, \quad A(x) = \begin{cases} +1, & x \in \Omega_+, \\ -1, & x \in \Omega_-, \end{cases}$$

where

$$\begin{aligned} \Omega_+ &= \{x \in \mathbb{R}^2 \mid \|x\| \leq R_1\} \cup \{x \in \mathbb{R}^2 \mid \|x\| \geq R_2\}, \\ \Omega_- &= \{x \in \mathbb{R}^2 \mid R_1 < \|x\| < R_2\} \end{aligned}$$

with $R_2 > R_1 > 0$. The quantity computed there for measuring the light propagation is the Dirichlet–to–Neumann–map for certain exterior domains. In the setting of the Sturm-Liouville theory the Dirichlet–to–Neumann–map is given by the Weyl-Titchmarsh m–function, which is also closely related to the scattering matrix. A generalization of the Weyl-Titchmarsh m–function to partial differential operators on exterior domains has been given recently by J. Behrndt and J. Rohleder in [13]. Such as in the one dimensional case, the generalization of the m–function is again the Dirichlet–to–Neumann–map. One can suspect that the generalization of the m–function is also closely related to the scattering matrix and to inverse scattering problems. A general relation between Dirichlet–to–Neumann–maps and scattering problems is not known to me, but in many specific situations there is a close relationship between both, see for example [78] and references given therein.

The analysis of the Dirichlet–to–Neumann–map in [22] leads G. Bouchitté and B. Schweizer to the interpretation that in the considered situation a cloaking phenomenon is taking place. Cloaking simplified means that there is an object in the system that can be made invisible for an observer looking at the system from outside. Of course, one can make any object invisible by putting it into a kind of box and decoupling the observer from the object of interest inside. Cloaking means rather that the measurement of the observer is the same in both cases, when the object is present and when it is not. Oversimplified one can say that cloaking means to hide something in a box, which is itself invisible.

Since at least in dimension $d = 1$ the Dirichlet–to–Neumann–map which is the measured quantity in [22] is related to scattering properties of the system it is reasonable to consider also scattering problems involving indefinite operators. The gluing formula given in Proposition 4.36 allows the qualitative analysis of the scattering properties of a quasi–one–dimensional system involving compact components, on which the operator is indefinite. In particular one can observe that even very small negative components have strong influence on the scattering matrix and new features arise, as the one discussed in Example 4.38. It is not clear if there is a relation to cloaking phenomena in higher dimensions. For a further investigation one can think of studying the behaviour of the scattering matrix, especially for small energies.

Part 2

Sign–indefinite forms and differential operators on bounded domains

The second part of the thesis is devoted to the study of differential operators $\mathcal{L}$ which are formally given by the differential expression

$$-\operatorname{div} A(\cdot) \operatorname{grad}$$

defined on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ and where the matrix valued function $A(\cdot)$ is not required to have constant sign. At $\partial\Omega$ Dirichlet boundary conditions are imposed. The motivation to consider these operators arises from models in optics as well as from solid-state physics. This has been carried out already in Chapter 4 of Part 1. In particular, optical metamaterials provide a possibility of constructing suitable devices making an object invisible, like the fabulous ‘invisibility cloak’ or ‘magic hat’ – *die Tarnkappe*. Due to this background the operator $\mathcal{L}$ is strikingly referred to as *magic hat operator*. An elementary example is the operator

$$\mathcal{L} = -\frac{d}{dx} \operatorname{sign}(x) \frac{d}{dx}$$

on a bounded interval with Dirichlet boundary conditions imposed at the endpoints. Such piecewise elliptic expressions have been studied in terms of extension theory in Chapter 4 already. In this part the approach using indefinite quadratic forms is taken on.

In Chapter 5 it is stated that under appropriate assumptions there is a unique self–adjoint indefinite operator $\mathcal{L}$ that is associated with the unbounded symmetric form $\mathfrak{l}$ defined by

$$\mathfrak{l}[v, u] = \langle \operatorname{grad} v, A(\cdot) \operatorname{grad} u \rangle_{L^2(\Omega)^d}, \quad \text{where } v, u \in H_0^1(\Omega) \subset L^2(\Omega).$$

The main concern of this part is the spectrum of such indefinite self–adjoint operators $\mathcal{L}$, and in particular the asymptotic distribution of their eigenvalues, which is discussed in Chapter 6.

The content of this part is mainly taken from the unpublished work [56] which is a joint work with Vadim Kostrykin, David Krejčiřík and Stephan Schmitz. It is supplemented with additional examples and a more detailed discussion of the asymptotic distribution of the eigenvalues.

CHAPTER 5

The magic hat operator

Consider in the Hilbert space $L^2(\Omega) \equiv L^2(\Omega;\mathbb{C})$ the densely defined unbounded sesquilinear form $\mathfrak{l}$ which is defined by

$$\mathfrak{l}[v,u] = \langle \operatorname{grad} v, A(\cdot) \operatorname{grad} u\rangle_{L^2(\Omega)^d} \quad \text{with } v,u \in H_0^1(\Omega) \subset L^2(\Omega),$$

where Ω is a bounded Lipschitz domain. If $A(x)$ is positive and Hermitian for almost every $x \in \Omega$ and $A(\cdot), A^{-1}(\cdot) \in L^\infty(\Omega;\mathbb{C})^{d\times d}$, the classical representation theorem, which is due to K. O. Friedrichs, applies, compare [58, Chapter VI], and see [17, §2] for the conditions on $A(\cdot)$. Consequently there is a unique self–adjoint operator associated with the form $\mathfrak{l}$, but what if $A(\cdot)$ is not sign–definite? The main difficulty then is the absence of coercivity in the unbounded form $\mathfrak{l}$. However there are generalizations of K. O. Friedrichs' representation theorem to indefinite quadratic forms. One formulation is given in the article [43], for further information on indefinite quadratic forms see also the references given therein. For a certain class of coefficient matrices one can overcome the difficulties arising from the absence of coercivity by the application of the mentioned representation theorem. From this the existence of a unique self–adjoint, boundedly invertible operator $\mathcal{L}$, associated with the form $\mathfrak{l}$ follows, just as in the classical case of closed semi–bounded forms. Furthermore, whenever the assumptions of the representation theorem are satisfied the spectrum of $\mathcal{L}$ is purely discrete and the two only accumulation points of the eigenvalues are $+\infty$ and $-\infty$. These results are formulated in Section 5.2.

After announcing results that are generalizations of or analogous to results obtained for operators associated with closed semi–bounded symmetric forms, one might be tempted to believe that the whole theory of sign–indefinite differential operators can be developed on the lines of the classical theory for elliptic operators. It turns out that the situation is not that simple, because form methods apply only under strong assumptions. These guarantee that the operator $\mathcal{L}$ is invertible and that its spectrum is discrete. However, when form methods do not apply directly, features appear that are particular to the indefinite case. The question, whether the assumptions of the representation theorem are fulfilled and the difficulties which arise are discussed in Section 5.3 of this chapter. Regularizations of the form $\mathfrak{l}$ are considered as well.

The construction of operators which are formally given by $-\operatorname{div} A(\cdot) \operatorname{grad}$ naturally involves the operators grad and div. Some preliminary facts are presented in the subsequent section. These are borrowed from the work [56] which is in preparation, and here most of them are given without proofs.

5.1. The operators div and grad

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with Lipschitz boundary. Denote by $C^\infty(\overline{\Omega})$ the set of complex valued functions which are smooth in Ω, and where all derivatives admit continuous prolongation to $\overline{\Omega} = \Omega \cup \partial\Omega$. With the scalar product $\langle \cdot, \cdot \rangle_{H^m(\Omega)}$ defined by

$$\langle u, v \rangle_{H^m(\Omega)} = \sum_{|i| \leq m} \int_\Omega \langle D^i u, D^i v \rangle, \quad \text{where } D^i u = \frac{d^{|i|} u}{dx_1^{i_1} dx_1^{i_2} \ldots dx_1^{i_N}}$$

for $i = (i_1, i_2, \ldots, i_N)$ and $|i| = i_1 + i_2 + \ldots + i_N$ the space $C^\infty(\overline{\Omega})$ becomes a pre–Hilbert space. The closure with respect to the Sobolev norm $\|\cdot\|_{H^m(\Omega)}$ defined by $\langle \cdot, \cdot \rangle_{H^m(\Omega)}$ is denoted $H^m(\Omega)$, compare for example [76, Chapter 1].

Denote by $C_0^\infty(\Omega)$ the set of smooth complex valued functions with compact support in Ω. With the scalar product $\langle \cdot, \cdot \rangle_{H_0^m(\Omega)}$ defined by

$$\langle u, v \rangle_{H_0^m(\Omega)} = \sum_{|i| = m} \int_\Omega \langle D^i u, D^i v \rangle$$

$C_0^\infty(\Omega)$ becomes a pre–Hilbert space the closure of which is denoted $H_0^m(\Omega)$, compare for example [76, Theorem 1.1].

Now, one considers the gradient operator D defined by

$$Du = \operatorname{grad} u, \qquad \text{for } u \in H_0^1(\Omega).$$

Some of the properties of D are summarized in the following

LEMMA 5.1. *The operator D is closed and its range $\operatorname{Ran}(D) \subset L^2(\Omega)^d$ is a closed subspace. Therefore $\operatorname{Ran} D$ is itself a Hilbert space with the Hilbert space structure inherited from $L^2(\Omega)^d$. Furthermore $\operatorname{Ker} D = \{0\}$ and in particular D as a map between Hilbert spaces*

$$D \colon H_0^1(\Omega) \to \operatorname{Ran} D$$

is bounded and boundedly invertible.

Consequently there is an orthogonal projector in $L^2(\Omega)^d$ onto $\operatorname{Ran} D$. This yields

LEMMA 5.2. *Let Ω be a bounded Lipschitz domain. Then*

$$Q \colon L^2(\Omega)^d \to \operatorname{Ran} D, \quad Qu := \begin{cases} u, & u \in \operatorname{Ran} D, \\ 0, & u \perp \operatorname{Ran} D \end{cases}$$

is a partial isometry.

Note that the adjoint operator $Q^* \colon \operatorname{Ran} D \to L^2(\Omega)^d$ is the embedding of $\operatorname{Ran} D$ into $L^2(\Omega)^d$.

PROOF OF LEMMA 5.1. The closeness of $\operatorname{Ran} D$ in $L^2(\Omega)^d$ is shown by the following argument. Let $v_j \in \operatorname{Ran} D$, $j \in \mathbb{N}$, with

$$v_j \to v \in L^2(\Omega)^d, \quad \text{where } v_j = \operatorname{grad} \varphi_j \text{ and } \varphi_j \in H_0^1(\Omega).$$

Hence,

$$\|\operatorname{grad} \varphi_j - \operatorname{grad} \varphi_k\|_{L^2(\Omega)^d} \to 0 \quad \text{for } j, k \to \infty.$$

From the Poincaré inequality, one obtains that

$$\begin{aligned}\|\varphi_j - \varphi_k\|^2_{H^1(\Omega)} &= \|\varphi_j - \varphi_k\|^2_{L^2(\Omega)} + \|\operatorname{grad}\varphi_j - \operatorname{grad}\varphi_k\|^2_{L^2(\Omega)^d} \\ &\leq (C_\Omega^2 + 1)\,\|\operatorname{grad}\varphi_j - \operatorname{grad}\varphi_k\|^2_{L^2(\Omega)^d} \to 0 \quad \text{for } j,k\to\infty,\end{aligned}$$

where C_Ω denotes the Poincaré constant of Ω. Hence, $(\varphi_j)_{j\in\mathbb{N}}$ is a Cauchy sequence in the Hilbert space $H^1(\Omega)$. Therefore, there exists a $\varphi\in H^1(\Omega)$ with $\|\operatorname{grad}\varphi_j - \operatorname{grad}\varphi\|_{H^1(\Omega)}\to 0$. Since $H^1_0(\Omega)$ is closed in $H^1(\Omega)$, one has $\varphi\in H^1_0(\Omega)$ and thus, $v = \operatorname{grad}\varphi\in\operatorname{Ran}D$. This proves both, that D is a closed operator and that $\operatorname{Ran}D\subset L^2(\Omega)^d$ is a closed subspace.

Since $|D| = (-\Delta_D)^{1/2}$, where $-\Delta_D = D^*D$ is the Dirichlet Laplacian one has that $|D|$ is injective and boundedly invertible as an operator in $L^2(\Omega)$. By the open mapping theorem the bounded map $D\colon H^1_0(\Omega)\to\operatorname{Ran}D$ is boundedly invertible. □

The adjoint of D is given by

$$D^*v = -\operatorname{div}v, \qquad v\in E^2(\Omega),$$

where

$$E^2(\Omega) := \{v\in L^2(\Omega)^d \,|\, \operatorname{div}v\in L^2(\Omega)\}.$$

Note that $H^1(\Omega)^d\subset E^2(\Omega)$ and that the set $E^2(\Omega)$ is the closure of $H^1(\Omega)^d$ with respect to the graph norm $(\|\cdot\|^2 + \|\operatorname{div}\cdot\|^2)^{1/2}$. If $d=1$, then even the equality $E^2(\Omega) = H^1(\Omega)$ holds. Recall that for domains Ω with Lipschitz boundary there exists a normal trace operator $\gamma_\nu : E^2(\Omega)\to H^{-1/2}(\partial\Omega)$ assigning to any $v\in E^2(\Omega)$ its normal component at the boundary, see [87, Lemma II.1.2.2]. The kernel of D^* is non–trivial. It is the orthogonal sum of the two closed subspaces

$$L^2_\sigma(\Omega)^d := \{v\in L^2(\Omega)^d \,|\, \operatorname{div}v = 0, \quad \gamma_\nu v = 0\}$$

and

$$H(\Omega) := \{v\in L^2(\Omega)^d \,|\, v = \operatorname{grad}\varphi, \quad \varphi\in H^1(\Omega), \quad \Delta\varphi = 0\},$$

see for example [28, Proposition IX.1.1]. The range of D^* is the whole of $L^2(\Omega)$. This follows already from the fact that the Dirichlet Laplacian $-\Delta_D = D^*D$ is surjective.

Since both D and D^* are closed operators, they admit polar decompositions, see for example [58, Section VI.2.7],

$$D = U|D| = |D^*|U \quad \text{and} \quad D^* = U^*|D^*| = |D|U^*, \tag{66}$$

where

$$U\colon L^2(\Omega)\to\operatorname{Ran}D$$

is a partial isometry with the initial subspace $(\operatorname{Ker}D)^\perp = L^2(\Omega)$ and the final subspace $\operatorname{Ran}D$. One can show that the partial isometry U maps $\operatorname{Dom}(D)$ onto $\operatorname{Dom}(D^*)\cap\operatorname{Ran}(D)$,

$$U\,|_{\operatorname{Dom}(D)}\colon\ \operatorname{Dom}(D)\to\operatorname{Ran}D\cap\operatorname{Dom}(D^*),$$

where $\operatorname{Dom}(D) = H^1_0(\Omega)$. This is going to be elaborated in [56].

REMARK 5.3. *From the properties of the partial isometry U it follows that* $\operatorname{Ran}D$ *is an invariant subspace of D^* and hence the operator D^* restricted to* $\operatorname{Ran}D\cap E^2(\Omega)$ *is unitarily equivalent to D. Consequently the operator D^* considered as a map between Hilbert spaces*

$$D^*\colon\ E^2(\Omega)\cap\operatorname{Ran}D\to L^2(\Omega)$$

is bounded and boundedly invertible.

5.2. Differential operators associated with indefinite quadratic forms

Consider the form $\mathfrak{l}$ defined by

$$\mathfrak{l}[v,u] = \langle \operatorname{grad} v, A(\cdot) \operatorname{grad} u\rangle_{L^2(\Omega)^d}, \qquad v,u \in H_0^1(\Omega) \subset L^2(\Omega). \tag{67}$$

For $A(x)$ positive and Hermitian almost everywhere in Ω such that $A(\cdot), A^{-1}(\cdot) \in L^\infty(\Omega;\mathbb{C})^{d\times d}$ this is a closed symmetric positive sesquilinear form, compare for example [17, §2]. The classical representation theorems apply and hence there is a unique self–adjoint operator $\mathcal{L} > 0$ associated to this form. What if $A(\cdot)$ is not sign–definite? The notion of closed forms is classically defined only for sectorial forms and particularly for symmetric semi–bounded forms, see [58, Chapter VI, §1.3]. However there is a generalization of closedness to non–sectorial or non–semi–bounded symmetric forms, see [75, Section 3]. Furthermore there are also generalizations of the classical representation theorems for symmetric and semi–bounded forms to non–semi–bounded symmetric forms; discussions and proofs can be found in the works [38,43] and [75].

Using the facts about D and D^* given in Section 5.1 one can adapt the form $\mathfrak{l}$ to the situation considered in the article [43]. There, operators of the form

$$\mathcal{B} = \mathcal{T}^{1/2} H \mathcal{T}^{1/2}$$

are considered, where H is a self–adjoint possibly sign-indefinite bounded and boundedly invertible operator, and the operator $\mathcal{T}$ is assumed to be self–adjoint positive and boundedly invertible.

Here, one considers the auxiliary operator

$$\mathcal{T} = QDD^*Q^*$$

in the Hilbert space $\operatorname{Ran} D$, which is self–adjoint and strictly positive, and the auxiliary form $\mathfrak{b}$ defined by

$$\mathfrak{b}[f,g] = \langle \mathcal{T}^{1/2} f, QM_A Q^* \mathcal{T}^{1/2} g\rangle_{\operatorname{Ran} D} \quad \text{with} \quad f,g \in \operatorname{Dom}(\mathcal{T}^{1/2}) \subset \operatorname{Ran} D,$$

where M_A denotes the multiplication operator with $A(\cdot)$, that is

$$M_A\colon L^2(\Omega)^d \to L^2(\Omega)^d, \quad M_A\phi = A(\cdot)\phi.$$

Note that $\mathcal{T}$ is unitarily equivalent to the Dirichlet Laplacian $-\Delta_D = D^*D$ in $L^2(\Omega)$. The crucial condition to apply the representation theorem [43, Theorem 2.3] to the form $\mathfrak{b}$, is that the operator $H = QM_AQ^*$ in the Hilbert space $\operatorname{Ran} D$ is boundedly invertible. This implies that $\mathfrak{b}$ is 0–closed in the notion introduced by A. G. R. McIntosh, see [75, Section 3], and consequently one also has that $\mathfrak{l}$ is 0–closed. Assuming this condition there is a unique self–adjoint invertible operator associated with the form $\mathfrak{b}$. Using further information from the operator theory of D and D^* yields that there is a unique self–adjoint invertible operator associated with the form $\mathfrak{l}$. This is going to be carried out in [56]. In this thesis only the resulting theorem is discussed, which is given here as Theorem 5.4. As already emphasized the assumptions of the forthcoming Theorem 5.4 do not require M_A to be sign-definite. Nonetheless, for $A(\cdot)$ such that M_A is sign–definite it reproduces the results of the classical theory.

THEOREM 5.4. *Let* $\Omega \subset \mathbb{R}^d$ *be a bounded Lipschitz domain and let* $A \in L^\infty(\Omega; \mathbb{C})^{d\times d}$ *be such that*

(a) $A(x)$ *is Hermitian for almost all* $x \in \Omega$,
(b) *the operator* $QM_AQ^* : \operatorname{Ran} D \to \operatorname{Ran} D$ *is boundedly invertible.*

Then

(i) *there exists a unique self-adjoint operator* $\mathcal{L}$ *with* $\operatorname{Dom}(\mathcal{L}) \subset H_0^1(\Omega)$ *such that*

$$\langle v, \mathcal{L}u\rangle_{L^2(\Omega)} = \langle \operatorname{grad} v, M_A \operatorname{grad} u\rangle_{L^2(\Omega)^d} \tag{68}$$

holds for all $v \in H_0^1(\Omega)$ *and all* $u \in \operatorname{Dom}(\mathcal{L})$. *Its domain is given by*

$$\operatorname{Dom}(\mathcal{L}) = \{u \in H_0^1(\Omega) \mid M_A Du \in E^2(\Omega)\}$$

and for any $u \in \operatorname{Dom}(\mathcal{L})$ *one has*

$$\mathcal{L}u = D^* M_A D u,$$

the domain $\operatorname{Dom}(\mathcal{L})$ *is a core for the gradient operator* D;

(ii) *the operator* $\mathcal{L}$ *is semi–bounded if and only if* QM_AQ^* *is sign–definite;*
(iii) $\mathcal{L}$ *is boundedly invertible with compact inverse. In particular, the spectrum of* $\mathcal{L}$ *is purely discrete.*

Roughly speaking, Theorem 5.4 states that the operator $\mathcal{L}$ is a self–adjoint realization of the formal differential expression $-\operatorname{div} A(\cdot) \operatorname{grad}$ with Dirichlet boundary conditions. In general, condition (b) in the assumptions of Theorem 5.4 is hard to verify. Only for $d = 1$ and under the additional assumption $A^{-1}(\cdot) \in L^\infty(\Omega; \mathbb{R})$, there is a complete spectral description of the operator QM_AQ^*. This is mainly due to the fact that for $d = 1$ one has $\operatorname{codim} \operatorname{Ran} D = 1$ and $(\operatorname{Ran} D)^\perp = \operatorname{Ker} D^*$ is spanned by the constant functions. In particular one gets

PROPOSITION 5.5. *Let* Ω *be a bounded open interval and* $A(\cdot), A(\cdot)^{-1} \in L^\infty(\Omega; \mathbb{R})$. *Then the operator* $QM_AQ^* : \operatorname{Ran} D \to \operatorname{Ran} D$ *is boundedly invertible if and only if*

$$\int_\Omega A(x)^{-1} dx \neq 0.$$

The proof is going to be carried out in [56] and is omitted here. The question when QM_AQ^* is invertible in higher dimensions cannot be answered in general. This constitutes an open problem which is discussed and described in Section 5.3. Proposition 5.12 indicates that the above Proposition 5.5 does not admit straightforward generalizations to dimensions $d \geq 2$.

EXAMPLE 5.6. *Consider an interval* $\Omega = (a, b)$ *and a measurable subset* $\Omega_+ \subset \Omega$. *Set* $\Omega_- = \Omega \setminus \Omega_+$ *and*

$$A(x) = \begin{cases} +1, & x \in \Omega_+, \\ -1, & x \in \Omega_-. \end{cases}$$

Assume that $|\Omega_-| \neq |\Omega_+|$. *Then applying Proposition 5.5 yields that the assumptions of Theorem 5.4 are satisfied and therefore* $\mathcal{L}$ *with its natural domain is self-adjoint and associated with the quadratic form given in* (67).

COROLLARY 5.7. *Let* $\mathcal{L}$ *be the operator constructed in Theorem 5.4. Then the inverse* $\mathcal{L}^{-1}$ *lies in the Schatten classes* $\mathfrak{S}_p$, *for* $p \geq \max\{2/d, 1\}$.

PROOF. Notice that from

$$\mathcal{L} = D^* M_A D = D^* Q M_A Q^* D$$

it follows that $\mathcal{L}^{-1}$ admits the representation

$$\mathcal{L}^{-1} = D^{-1}(Q M_A Q^*)^{-1}(D^*)^{-1},$$

where D^{-1} is regarded as a map from $\operatorname{Ran}(D)$ to $H_0^1(\Omega) \subset L^2(\Omega)$ and $(D^*)^{-1}$ is considered as a map from $L^2(\Omega)$ to $\operatorname{Ran} D$, compare Lemma 5.1 and Remark 5.3, respectively. By assumption (b) of Theorem 5.4 the operator $Q M_A Q^*$ as a map in $\operatorname{Ran} D$ is boundedly invertible. Note that $|D|^{-2} = (D^* D)^{-1} \in \mathfrak{S}_p$ for $p \geq 2/d$, which follows from the classical Weyl law for the Dirichlet Laplacian on bounded domains, see [94]. For the singular values of compact operators one has the equality $s_j(D^{-1}) = s_j\left((D^*)^{-1}\right)$, $j \in \mathbb{N}$, see for example [40, Chapter II, §2, equation (2.1)]. Therefore also $|D^*|^{-2} \in \mathfrak{S}_p$ for $p \geq 2/d$. As $(Q M_A Q^*)^{-1}$ is bounded one has that $(Q M_A Q^*)^{-1}(D^*)^{-1} \in \mathfrak{S}_{2p}$ and applying [40, Theorem 7.1, Chapter III], gives that $\mathcal{L}^{-1} = D^{-1}(Q M_A Q^*)^{-1}(D^*)^{-1} \in \mathfrak{S}_p$ for $p \geq 2/d$ with $p \geq 1$. □

Regularized problems. Instead of considering the form $\mathfrak{l}$ one can consider regularized problems related to forms $\mathfrak{l}(\epsilon)$, which are defined by

$$\mathfrak{l}(\epsilon)[u,v] := \langle Du, M_{A(\epsilon)} Dv \rangle_{L^2(\Omega)^d}, \quad u, v \in H_0^1(\Omega) \subset L^2(\Omega),$$

where

$$A(\epsilon)(x) = A(x) + i\epsilon, \quad \text{for } \epsilon > 0 \text{ and } x \in \Omega.$$

The numerical range of $\mathfrak{l}(\epsilon)$ lies in a sector in the upper half plane of $\mathbb{C}$. Rotating the form by $\pi/2$ to the right, by multiplying with minus the imaginary unit $-i$ one obtains a closed sectorial form. Hence the classical representation theorem applies to $\mathfrak{l}(\epsilon)$ and there is a unique closed non–self–adjoint operator $\mathcal{L}_\varepsilon$ associated with $\mathfrak{l}(\epsilon)$. Since $Q M_A Q^*$ is a bounded self-adjoint operator in $\operatorname{Ran} D$ the regularization

$$Q M_{A(\epsilon)} Q^* = Q M_A Q^* + i\epsilon Q Q^*,$$

is invertible for any $\epsilon > 0$ and $\mathcal{L}_\varepsilon$ becomes more concretely

$$\mathcal{L}_\epsilon = D^* M_{A(\epsilon)} D$$

with compact inverse

$$\mathcal{L}_\epsilon^{-1} = D^{-1}(Q M_{A(\epsilon)} Q^*)^{-1}(D^*)^{-1}.$$

COROLLARY 5.8. *Let $\mathcal{L}_0 := \mathcal{L}$ be the operator constructed in Theorem 5.4. Then*

$$\|\mathcal{L}_\epsilon^{-1} - \mathcal{L}_0^{-1}\| \to 0, \quad \textit{for} \quad \epsilon \to 0,$$

where $\|\cdot\|$ denotes the operator norm in $L^2(\Omega)$.

Note that the regularized problem can be formulated always in bounded Lipschitz domains, since $Q M_{A(\epsilon)} Q^*$ is boundedly invertible for any $\epsilon > 0$. However the proof of the convergence proposed here is valid only if the limit operator $Q M_{A(0)} Q^* = Q M_A Q^*$ is boundedly invertible as well.

PROOF OF COROLLARY 5.8. For $\epsilon > 0$ sufficiently small one has the Neumann series representation

$$(QM_{A(\epsilon)}Q^*)^{-1} = (QM_A Q^*)^{-1} \left(\mathbb{1}_{\operatorname{Ran} D} + \sum_{n=1}^{\infty} (i\epsilon)^n (QM_A Q^*)^{-n} \right),$$

where

$$\sum_{n=1}^{\infty} (i\epsilon)^n (QM_A Q^*)^{-n} \to 0 \qquad \text{for} \quad \epsilon \to 0,$$

in the operator norm topology. Consequently

$$\|(QM_{A(\epsilon)}Q^*)^{-1} - (QM_A Q^*)^{-1}\| \to 0, \quad \text{for} \quad \epsilon \to 0.$$

As the operators D^{-1} and $(D^*)^{-1}$ are bounded, compare Lemma 5.1 and Remark 5.3, it follows that

$$\mathcal{L}_\epsilon^{-1} - \mathcal{L}^{-1} = D^{-1} \left[(QM_{A(\epsilon)}Q^*)^{-1} - (QM_A Q^*)^{-1} \right] (D^*)^{-1} \to 0, \quad \text{for} \quad \epsilon \to 0$$

with respect to the operator norm topology. □

In specific situations other regularizations can be considered also.

REMARK 5.9. *Assume that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain and suppose that there are non–empty open sets $\Omega_\pm \subset \Omega$ such that*

$$\Omega_- \cap \Omega_+ = \emptyset \quad \textit{and} \quad \overline{\Omega_-} \cup \overline{\Omega_+} = \overline{\Omega}.$$

Consider the regularized coefficient

$$\widetilde{A}(\epsilon)(x) = \begin{cases} +\mathbb{1}, & x \in \Omega_+, \\ -\mathbb{1} + i\epsilon, & x \in \Omega_-. \end{cases}$$

Let $\widetilde{\mathfrak{l}}(\epsilon)$ be the form which is given by

$$\widetilde{\mathfrak{l}}(\epsilon)[u,v] := \langle Du, M_{\widetilde{A}(\epsilon)} Dv \rangle_{L^2(\Omega)^d} \quad u, v \in H_0^1(\Omega) \subset L^2(\Omega).$$

By rotating $\widetilde{\mathfrak{l}}(\epsilon)$ one can obtain a closed sectorial form, which by the classical results defines uniquely the closed non–self–adjoint operator

$$\widetilde{\mathcal{L}}_\epsilon = D^* M_{\tilde{A}(\epsilon)} D.$$

Such operators have been considered in the context of metamaterials, compare for example the article [22] and the references cited therein. Assume that $QM_{\widetilde{A}(0)}Q^*$ is boundedly invertible and let $\widetilde{\mathcal{L}}_0 := \mathcal{L}$ be the operator constructed in Theorem 5.4. Analogously to Corollary 5.8 one proves now

$$\|\widetilde{\mathcal{L}}_\epsilon^{-1} - \tilde{\mathcal{L}}_0^{-1}\| \to 0, \quad \textit{for} \quad \epsilon \to 0,$$

where one applies that

$$QM_{\widetilde{A}(\epsilon)}Q^* = QM_{\widetilde{A}(0)}Q^* + i\epsilon\, Q\chi_{\Omega_-}Q^*, \quad \chi_{\Omega_-}(x) = \begin{cases} \mathbb{1}, & x \in \Omega_-, \\ 0, & \textit{else} \end{cases}$$

is boundedly invertible for $\epsilon > 0$ small enough.

The convergence of the eigenvalues and eigenfunctions in $L^2(\Omega)$ of the regularizations proposed in Corollary 5.8 and Remark 5.9 follows from norm convergence of the regularized operators. Note that for the proof of the convergence of the regularized operators given here, it is crucial to assume that the limit operator $QM_{A(0)}Q^*$ is boundedly invertible. This assures that the limit differential operator $\mathcal{L}$ along with the regularizations $\mathcal{L}_\epsilon$ and $\tilde{\mathcal{L}}_\epsilon$, respectively can be defined using form methods. Using Corollary 5.7 one can prove in Corollary 5.8 and Remark 5.9 even convergence in an appropriate Schatten norm.

In the article [21] another approach is elaborated to overcome the difficulties arising from the absence of coercivity in the unbounded form $\mathfrak{l}$. This approach uses the concept of *T–coercivity*. The relation between T–coercive forms and the indefinite forms discussed in Theorem 5.4 needs further investigation.

5.3. The operator QM_AQ^* – an open problem

The operator QM_AQ^* plays an important role in the proof of Theorem 5.4 and in the understanding of the operator theory of differential operators of the type D^*M_AD. As QM_AQ^* is bounded in the Hilbert space $\operatorname{Ran} D$, the operator QM_AQ^* itself can be tackled using sesquilinear forms. It is uniquely defined by the bounded symmetric form $\mathfrak{a}$ which is given by

$$\mathfrak{a}[\psi,\varphi] = \langle \psi, M_A\varphi\rangle_{\operatorname{Ran} D} \quad \text{with } \psi,\varphi \in \operatorname{Ran} D. \tag{69}$$

Equivalently one can consider the bounded sesquilinear form $\mathfrak{a}_D$ defined by

$$\mathfrak{a}_D[u,v] = \langle Du, M_ADv\rangle_{L^2(\Omega)^d}, \quad u,v \in H_0^1(\Omega),$$

in the Hilbert space $H_0^1(\Omega)$ with scalar product $\langle\cdot,\cdot\rangle_{H_0^1(\Omega)} = \langle\cdot,\cdot\rangle_D = \langle D\cdot, D\cdot\rangle_{L^2(\Omega)^d}$. The form $\mathfrak{a}_D$ looks formally like $\mathfrak{l}$, but one has to take into account that for $\mathfrak{a}_D$ – since it is a form in the Hilbert space $H_0^1(\Omega)$ – a normalized vector satisfies $\|Du\|_{L^2(\Omega)^d} = 1$, whereas $\mathfrak{l}$ is an unbounded form in the Hilbert space $L^2(\Omega)$, where the normalization is $\|u\|_{L^2(\Omega)} = 1$. The relation between both $\mathfrak{a}$ and $\mathfrak{a}_D$ is specified in

REMARK 5.10. *The form $\mathfrak{a}_D[\cdot,\cdot]$ defines uniquely the bounded operator $D^{-1}QM_AQ^*D$ in the Hilbert space $H_0^1(\Omega)$, equipped with the scalar product $\langle\cdot,\cdot\rangle_D = \langle D\cdot, D\cdot\rangle_{L^2(\Omega)^d}$. This operator is unitarily equivalent to the operator QM_AQ^* defined by the form $\mathfrak{a}$ in $\operatorname{Ran} D$. This follows from the fact that the Hilbert spaces $\operatorname{Ran} D$ and $H_0^1(\Omega)$ are isometrically isomorph, where the isomorphism is given by the boundedly invertible map $D\colon H_0^1(\Omega) \to \operatorname{Ran} D$, compare Lemma 5.1.*

The problem of verifying whether the operator QM_AQ^* is boundedly invertible is particular to the case of coefficients $A(\cdot)$, where M_A is not sign–definite. This follows from the subsequent

PROPOSITION 5.11. *Let Ω be a bounded Lipschitz domain and assume that $A(x)$ is positive and Hermitian almost everywhere in Ω, and $A(\cdot), A^{-1}(\cdot) \in L^\infty(\Omega;\mathbb{C})^{d\times d}$. Then the operator QM_AQ^* is boundedly invertible.*

PROOF. From the assumptions it follows that M_A is positive and Hermitian in $L^2(\Omega)^d$. The statement is implied by the inequality

$$\inf_{\substack{\psi\in\operatorname{Ran} D\\ \|\psi\|=1}} \langle\psi, M_A\psi\rangle_{L^2(\Omega)^d} \geq \inf_{\substack{\varphi\in L^2(\Omega)^d\\ \|\varphi\|=1}} \langle\varphi, M_A\varphi\rangle_{L^2(\Omega)^d} \geq c, \quad \text{where } c = \|A(\cdot)^{-1}\|_\infty^{-1} > 0,$$

since the spectrum of QM_AQ^* is contained in the numerical range. □

If M_A is sign–indefinite then the invertibility of QM_AQ^* can no longer be taken for granted. In the subsequent two subsections examples of non–invertible and invertible QM_AQ^* are discussed. Unfortunately for dimension $d \geq 2$ there is no general criterion known to me that would assure the bounded invertibility of the operator QM_AQ^*.

5.3.1. Non–invertible QM_AQ^*. The constant coefficient matrix

$$A = \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix} \tag{70}$$

is in some sense the worst case.

PROPOSITION 5.12. *Let $x = (x_1, x_2) \in \Omega = (0, a) \times (0, b)$ and $A(x) = A$ be given by* (70). *Then the spectrum of QM_AQ^* is*

$$\sigma(QM_AQ^*) = [-1, 1].$$

The spectral gap of M_A, which has in its spectrum only the two points $+1$ and -1, is closed entirely for QM_AQ^*. This underlines that assumption (b) in Theorem 5.4 is not self–evident in general.

PROOF. In the considered situation one can work with a very explicit basis of $\operatorname{Ran} D$. The functions

$$\phi_{n,m}(x_1, x_2) = \sin\left(\frac{\pi n}{a} x_1\right) \cdot \sin\left(\frac{\pi m}{b} x_2\right), \qquad n, m \in \mathbb{N}$$

are the eigenfunctions of the Dirichlet Laplacian $-\Delta_D = D^*D$ and therefore they form an orthogonal basis of $L^2(\Omega)$. Since the operator $-\Delta_D$ is defined uniquely by the closed symmetric strictly positive form given by

$$\langle \operatorname{grad} u, \operatorname{grad} v \rangle_{L^2(\Omega)^d} \quad \text{with } u, v \in H_0^1(\Omega) \subset L^2(\Omega),$$

the functions

$$\psi_{n,m} := \frac{D\phi_{n,m}}{\|D\phi_{n,m}\|}, \qquad n, m \in \mathbb{N},$$

form an orthonormal basis of the Hilbert space $\operatorname{Ran} D$. Inserting this into the form $\mathfrak{a}$ gives an infinite dimensional matrix representation of the operator QM_AQ^* with entries

$$(QM_AQ^*)_{(n,m),(k,l)} = \langle \psi_{n,m}, M_A \psi_{k,l} \rangle.$$

Analogously one obtains for the shifted operator $QM_AQ^* - \lambda$ with $\lambda \in \mathbb{C}$ the matrix with entries

$$(QM_AQ^* - \lambda)_{(n,m),(k,l)} = \langle \psi_{n,m}, (A - \lambda)\, \psi_{k,l} \rangle,$$

where $(n, m), (k, l) \in \mathbb{N}^2$. Set

$$\mu_{(n,m),(k,l)}[\lambda] := (QM_AQ^* - \lambda)_{(n,m),(k,l)}$$

and note that

$$\mu_{(n,m),(k,l)}[\lambda] = \delta_{(n,m),(k,l)} \frac{(1-\lambda)\frac{m^2}{a^2} - (1+\lambda)\frac{n^2}{b^2}}{\frac{m^2}{a^2} + \frac{n^2}{b^2}},$$

where $\delta_{(n,m),(k,l)}$ is the Kronecker-delta for the multi-indices $(n, m), (k, l) \in \mathbb{N}^2$. Thus $QM_AQ^* - \lambda$ has been represented by a diagonal matrix with diagonal entries $\mu_{(n,m),(n,m)}[\lambda]$ and consequently the spectrum of $QM_AQ^* - \lambda = QM_{A-\lambda}Q^*$ is the closure of the matrix' diagonal entries. Assume that $\lambda \in (-1, 1)$, then for $(n, m) \in \mathbb{N}^2$

$$\mu_{(n,m),(n,m)}[\lambda] = n^2 \left[\frac{m}{n} - \frac{a}{\sqrt{1-\lambda}} \frac{\sqrt{1+\lambda}}{b} \right] \left[\frac{m\frac{\sqrt{1-\lambda}}{a} + n\frac{\sqrt{1+\lambda}}{b}}{n\frac{a}{\sqrt{1-\lambda}}\left(\frac{m^2}{a^2} + \frac{n^2}{b^2}\right)} \right]. \tag{71}$$

From the equivalence of norms in $\mathbb{R}^2$ it follows that there is a constant $C_{a,b,\lambda} > 0$ such that for the second factor on the right hand side of equation (71)

$$\frac{m\frac{\sqrt{1-\lambda}}{a} + n\frac{\sqrt{1+\lambda}}{b}}{n\frac{a}{\sqrt{1-\lambda}}\left(\frac{m^2}{a^2} + \frac{n^2}{b^2}\right)} \le \frac{C_{a,b,\lambda}}{n\sqrt{n^2+m^2}}$$

holds. By Hurwitz's theorem, see [49, Theorem 1], for any real numbers $r \in \mathbb{R}$ and $l \in \mathbb{R} \setminus \{0\}$ one has

$$c(r/l) := \liminf_{\substack{\|(n,m)\| \to \infty \\ n,m \in \mathbb{N}}} n^2 \left| \frac{m}{n} - \frac{r}{l} \right| \le \frac{1}{\sqrt{5}}, \tag{72}$$

and therefore $c(r/l)$ is uniformly bounded. Here one takes

$$r = \frac{a}{\sqrt{1-\lambda}} \quad \text{and} \quad l = \frac{b}{\sqrt{1+\lambda}}.$$

Consequently there exists a sequence $\{(n_j, m_j)\}_{j \in \mathbb{N}}$, where $n_j, m_j \in \mathbb{N}$, such that for the first factor on the right hand side of equation (71) one has

$$n_j^2 \left| \frac{m_j}{n_j} - \frac{a}{\sqrt{1-\lambda}} \frac{\sqrt{1+\lambda}}{b} \right| \le \frac{1}{\sqrt{5}},$$

whereas the second factor on the right hand side of equation (71) goes to zero for $j \to \infty$. Putting the two pieces together one obtains that for $\lambda \in (-1, 1)$

$$(QM_AQ^* - \lambda)_{(n_j,m_j),(n_j,m_j)} \to 0, \quad \text{for} \quad j \to \infty.$$

This means that zero is an accumulation point of the eigenvalues of $QM_AQ^* - \lambda$. Hence zero is in the spectrum of $QM_AQ^* - \lambda$ for any $\lambda \in (-1, 1)$. As the spectrum is a closed set the claim follows. □

Nevertheless, in the situation described in Proposition 5.12 one can construct a self–adjoint realization of

$$-\mathrm{div}\, A\, \mathrm{grad} = -\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2}.$$

This is done by proposing a complete orthogonal basis of eigenvectors to real eigenvalues. The spectral resolution is usually obtained from a given self–adjoint operator, here the procedure is the other way around.

Consider the functions $\phi_{n,m}$ with $n, m \in \mathbb{N}$. These are the eigenfunctions of the Dirichlet Laplacian $-\Delta_D = D^*D$ and hence they form a complete basis of orthogonal functions in $L^2(\Omega)$. One has

$$-\left(\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2}\right)\phi_{n,m} = \left[\left(\frac{\pi n}{a}\right)^2 + \left(\frac{\pi m}{b}\right)^2\right]\phi_{n,m}$$

and furthermore

$$\left(-\frac{d^2}{dx_1^2}+\frac{d^2}{dx_2^2}\right)\phi_{n,m}=\left[\left(\frac{\pi n}{a}\right)^2-\left(\frac{\pi m}{b}\right)^2\right]\phi_{n,m}.$$

Hence one has a complete orthogonal basis of eigenfunctions to real eigenvalues, and consequently these define a self–adjoint operator $\mathcal{L}'$. More precisely $\mathcal{L}'$ is defined on $L^2(\Omega)$ by

$$\mathcal{L}'u=\sum_{n,m\in\mathbb{N}}\lambda_{n,m}\frac{\phi_{n,m}}{\|\phi_{n,m}\|}\left\langle u,\frac{\phi_{n,m}}{\|\phi_{n,m}\|}\right\rangle_{L^2(\Omega)}$$

on its natural domain, where

$$\lambda_{n,m}=\left(\frac{\pi n}{a}\right)^2-\left(\frac{\pi m}{b}\right)^2,\quad \text{for } n,m\in\mathbb{N}.$$

The spectrum of $\mathcal{L}'$ consists of the closure of the set of eigenvalues

$$\sigma(\mathcal{L}')=\mathrm{clo}\,\{\lambda_{n,m}\mid n,m\in\mathbb{N}\}$$

and it shows some interesting features, which have been observed by V. Kostrykin. The number a/b is called a badly approximable irrational number, if the quantity $c(a/b)$ defined in equation (72) is larger than zero.

LEMMA 5.13. *Let a/b be badly approximable. Then for arbitrary δ with $c(a/b)>\delta>0$ there is at most a finite number of pairs $(n,m)\in\mathbb{N}^2$ such that*

$$n^2\left|\frac{a}{b}-\frac{m}{n}\right|<c(a/b)-\delta. \tag{73}$$

PROOF. Suppose there is infinite number of pairs (n_k,m_k) satisfying (73). Then

$$\liminf_{k\to\infty} m_k\,|m_ka/b-n_k|\le c(x)-\delta,$$

which contradicts to (72). □

Write

$$\lambda_{n,m}=\pi^2\left(\frac{n^2}{a^2}-\frac{m^2}{b^2}\right)=\frac{\pi^2m^2}{a^2}\left(\frac{n}{m}-\frac{a}{b}\right)\left(\frac{n}{m}+\frac{a}{b}\right),\quad n,m\in\mathbb{N}.$$

If the quotient a/b is rational, $\mathcal{L}'$ has the eigenvalue zero of infinite multiplicity.

If a/b is a well approximable irrational number, that is a/b is not rational, but $c(a/b)=0$, then zero is in the essential spectrum of $\mathcal{L}$, since

$$m^2\left(\frac{n}{m}-\frac{a}{b}\right),\quad n,m\in\mathbb{N},$$

can be made arbitrary small.

Assume now that a/b is a badly approximable irrational number. Then zero is not an eigenvalue of $\mathcal{L}'$. Moreover,

$$|\lambda_{n,m}|\ge\frac{\pi^2}{ab}m^2\left|\frac{n}{m}-\frac{a}{b}\right|.$$

By Lemma 5.13,

$$m^2\left|\frac{n}{m}-\frac{a}{b}\right|\ge c(a/b)-\delta$$

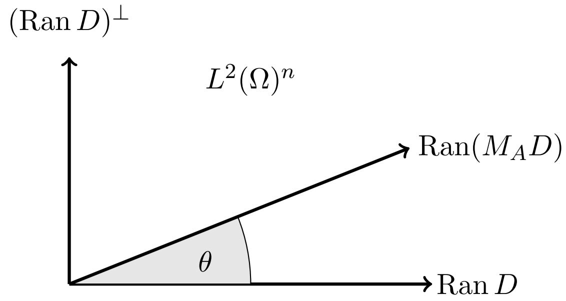


FIGURE 8. $\operatorname{Ran}(M_A D)$ as a subspace of $L^2(\Omega)^d = \operatorname{Ran} D \oplus (\operatorname{Ran} D)^{\perp}$ and the angle $\theta = \sphericalangle(\operatorname{Ran} D, \operatorname{Ran}(M_A D))$.

holds for all $(n, m) \in \mathbb{N}^2$ except for an finite number of pairs (n, m). Hence, $\mathcal{L}'$ is even boundedly invertible. However, in all three cases, by Proposition 5.12 the operator $\mathcal{L}'$ does not fit into the framework of Theorem 5.4. Nonetheless one has

LEMMA 5.14. *The closure of $D^* M_A D$ is the operator $\mathcal{L}'$, and therefore $D^* M_A D$ is essentially self–adjoint.*

The operator $D^* M_A D$ is the composition of the unbounded operator D, the bounded operator M_A and the unbounded operator D^*. The operator $D^* M_A D$ fails to be self–adjoint. It is only essentially self-adjoint. This is due to the fact that its domain is contained by construction in $H_0^1(\Omega)$, and for the compact embedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ it would have compact resolvent if it were self–adjoint. However, by the above reasoning the spectrum of $\mathcal{L}'$ is not purely discrete. Also, Theorem 5.4 does not apply and therefore the relation of $\mathcal{L}'$ to the form $\mathfrak{l}$ is unclear. In particular, it is unclear whether $\operatorname{Dom}(\mathcal{L}')$ is a core for the gradient operator D.

Summarizing one can say that in the situations where Theorem 5.4 applies the operator $\mathcal{L}$ keeps many properties known from the sign–definite elliptic operators on bounded domains like the compactness of the resolvent and some of the relations to forms. If Theorem 5.4 does not apply it can still be possible to construct at least essentially self–adjoint operators formally given by $-\operatorname{div} A(\cdot) \operatorname{grad}$ with domain in $H_0^1(\Omega)$, but the behaviour of their spectrum cannot be predicted and the relation to the corresponding form is unclear.

PROOF OF LEMMA 5.14. It is sufficient to prove the equality on a complete orthogonal basis of $L^2(\Omega)$. The functions $\phi_{n,m}$ are clearly in $\operatorname{Dom}(D)$, furthermore $M_A D \phi_{n,m} \in E^2(\Omega)$ and $D^* M_A D \phi_{n,m} = \lambda_{n,m} \phi_{n,m}$, which proves the claim. $\square$

An illustration of the invertiblility of $Q M_A Q^*$ can be provided in terms of a geometric interpretation of the space $\operatorname{Ran}(M_A D)$ considered as a subspace of

$$L^2(\Omega)^d = \operatorname{Ran} D \oplus (\operatorname{Ran} D)^{\perp}.$$

The operator Q acts as the orthogonal projection in $L^2(\Omega)^d$ onto $\operatorname{Ran} D$ restricted to its range. Hence the operator $Q M_A Q^*$ is boundedly invertible whenever the angle between the spaces $\operatorname{Ran}(M_A D) \subset L^2(\Omega)^d$ and $\operatorname{Ran} D \subset L^2(\Omega)^d$ is smaller than $\pi/2$. Equivalently one has that $Q M_A Q^*$ is boundedly invertible whenever the angle between the spaces $\operatorname{Ran}(M_A D) \subset L^2(\Omega)^d$ and $(\operatorname{Ran} D)^{\perp} \subset L^2(\Omega)^d$ is larger zero. The cosine of the angle between the subspaces

$\operatorname{Ran} D$ and $\operatorname{Ran}(M_A D)$ is

$$\cos\left(\sphericalangle\left(\operatorname{Ran} D, \operatorname{Ran}(M_A D)\right)\right) = \inf_{\|Du\|=1} \sup_{\|M_A Dv\|=1} |\langle Du, M_A Dv\rangle|.$$

This criterion for the invertibility of QM_AQ^* implies the weak coercitivity of the form $\mathfrak{a}$ defined by (69). The generalization due to I. Babushka of the Lax-Milgram Theorem given in [9] states that weakly coercive bounded forms define bounded and boundedly invertible operators.

REMARK 5.15. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Assume that there is a solution u_0 to the differential equation*

$$-\operatorname{div} A(\cdot) \operatorname{grad} u_0 = 0 \quad \text{with } u_0 \in H_0^1(\Omega).$$

Then $A(\cdot) \operatorname{grad} u_0 \in E^2(\Omega)$ and furthermore $A(\cdot) \operatorname{grad} u_0 \in \operatorname{Ker} D^*$, which implies $A(\cdot) \operatorname{grad} u_0 \perp \operatorname{Ran} D$. Hence $Du_0 \in \operatorname{Ker} QM_AQ^*$ and the angle between $\operatorname{Ran} D$ and $\operatorname{Ran}(M_A D)$ is $\pi/2$ and therefore the operator QM_AQ^* fails to be boundedly invertible.

EXAMPLE 5.16. *Consider for $x = (x_1, x_2) \in \Omega = (-a, a) \times (0, 1)$ the coefficients $A(x) = \operatorname{sign}(x_1) \cdot \mathbb{1}$. Then the functions*

$$u_m(x_1, x_2) = \phi_m(x_1) \cdot \sin(m\pi x_2), \quad m \in \mathbb{N},$$

where

$$\phi_m(x_1) = \begin{cases} \sinh((\pi m)(a - x)), & x \in (0, a), \\ \sinh((\pi m)(x + a)), & x \in (-a, 0), \end{cases}$$

are elements of $H_0^1(\Omega)$, and each u_m solves the equation

$$-\operatorname{div} A(\cdot) \operatorname{grad} u_m = 0$$

referred to in Remark 5.15. Consequently $Du_m \in \operatorname{Ker} QM_AQ^*$ and the operator QM_AQ^* is not boundedly invertible. Again one can define $\mathcal{L}' = \overline{D^* M_A D}$ and one obtains that zero is an eigenvalue of $\mathcal{L}'$ of infinite multiplicity.

5.3.2. Examples where the operator QM_AQ^* is invertible. In order to construct a class of examples where QM_AQ^* is boundedly invertible and sign–indefinite, one can consider a highly symmetric situation where one is able to determine the spectrum of QM_AQ^*. It is going to turn out that the spectrum has a gap then, and therefore one can consider the shifted operator $QM_AQ^* - \lambda = QM_{(A-\lambda)}Q^*$ for appropriate $\lambda \in \mathbb{R}$.

A domain $\Omega \subset \mathbb{R}^d$ is called *symmetric with respect to x_1* if one has

$$x = (x_1, x_2, \ldots, x_d) \in \Omega \quad \text{if and only if} \quad (-x_1, x_2, \ldots, x_d) \in \Omega.$$

This means Ω is symmetric with respect to the $(d-1)$–dimensional hypersurface with $x_1 = 0$.

PROPOSITION 5.17. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain which is symmetric with respect to x_1. Assume furthermore that the domains*

$$\Omega_+ = \{x \in \Omega \mid x_1 > 0\} \quad \text{and} \quad \Omega_- = \{x \in \Omega \mid x_1 < 0\}$$

are Lipschitz too, and consider

$$A(x) = \operatorname{sign}(x_1) \cdot \mathbb{1}.$$

Then

$$\{-1, 1\} \subset \sigma(QM_AQ^*) \subset \{-1, 0, 1\}.$$

From this one obtains immediately by a scaling argument

COROLLARY 5.18. *Let* $\Omega_+, \Omega_-, \Omega \subset \mathbb{R}^d$ *be as in Proposition 5.17 and let be* $c_+ > 0$ *and* $c_- < 0$ *with* $|c_-| \neq |c_+|$. *Then for*

$$A(x) = \begin{cases} c_+ \mathbb{1}, & \text{for } x \in \Omega_+, \\ c_- \mathbb{1}, & \text{for } x \in \Omega_- \end{cases}$$

the operator QM_AQ^* *is boundedly invertible and sign–indefinite.*

The above corollary delivers a class of examples in dimension $d \geq 2$ for which Theorem 5.4 is applicable. For the situation described in Corollary 5.18 it has been shown in [21, Theorem 3.1] that the form $\mathfrak{l}$ is T–coercive.

PROOF OF PROPOSITION 5.17. The proof of Proposition 5.17 takes advantage of the given symmetries. Since Ω is symmetric with respect to x_1 one can introduce the following notions. A function $v \in H_0^1(\Omega)$ is called *odd with respect to* x_1 if

$$v(x_1, x_2, \dots, x_d) = -v(-x_1, x_2, \dots, x_d)$$

and $v \in H_0^1(\Omega)$ is called *even with respect to* x_1 if

$$v(x_1, x_2, \dots, x_d) = v(-x_1, x_2, \dots, x_d).$$

Note that for any function $v \in H_0^1(\Omega)$

$$v^{odd}(x) = \frac{1}{2}\big\{v(x_1, x_2, \dots, x_d) - v(-x_1, x_2, \dots, x_d)\big\}$$

defines a function v^{odd} which is odd with respect to x_1 and

$$v^{even}(x) = \frac{1}{2}\big\{v(x_1, x_2, \dots, x_d) + v(-x_1, x_2, \dots, x_d)\big\}$$

defines a function v^{even} which is even with respect to x_1. Furthermore one has for any $v \in H_0^1(\Omega)$

$$v = v^{odd} + v^{even}.$$

This gives rise to the definition of

$$H_0^1(\Omega)^{even} := \{v \in H_0^1(\Omega) \mid v \text{ even with respect to } x_1\}$$

and

$$H_0^1(\Omega)^{odd} := \{v \in H_0^1(\Omega) \mid v \text{ odd with respect to } x_1\},$$

which are both closed subspaces of $H_0^1(\Omega)$. Observe that $v \in H_0^1(\Omega)^{even}$ if and only if $v = v^{even}$ and $v \in H_0^1(\Omega)^{odd}$ if and only if $v = v^{odd}$. Furthermore

$$H_0^1(\Omega)^{even} \cap H_0^1(\Omega)^{odd} = \{0\}$$

and consequently one has the decomposition into the direct sum

$$H_0^1(\Omega) = H_0^1(\Omega)^{even} \oplus H_0^1(\Omega)^{odd}. \tag{74}$$

Now, one investigates the behaviour of $H_0^1(\Omega)^{even}$ and $H_0^1(\Omega)^{odd}$ under the action of the gradient operator D. By the chain rule

$$Dv^{odd}(x) = \frac{1}{2}\big\{(Dv)(x_1, x_2, \dots, x_d) - J(Dv)(-x_1, x_2, \dots, x_d)\big\}, \quad \text{for } v \in H_0^1(\Omega),$$

where $J = \operatorname{diag}\{-1, +1, \dots, +1\}$ is a $d \times d$–diagonal matrix. Hence the first component $\left(Dv^{odd}\right)_1$ is almost everywhere in Ω even with respect to x_1, whereas the other components $\left(Dv^{odd}\right)_j$ with $j = 2, \dots, d$ are almost everywhere in Ω odd with respect to x_1. Analogously one obtains

$$Dv^{even}(x) = \frac{1}{2}\big\{(Dv)(x_1, x_2, \dots, x_d) + J(Dv)(-x_1, x_2, \dots, x_d)\big\}$$

and hence the first component $(Dv^{even})_1$ is almost everywhere in Ω odd with respect to x_1, whereas the other components $(Dv^{even})_j$ with $j = 2, \dots, d$ are almost everywhere in Ω even with respect to x_1. One has the following elementary

LEMMA 5.19. *Let $\Omega \subset \mathbb{R}^d$ be symmetric with respect to x_1 and let $\varphi, \psi \in L^2(\Omega)$. Assume that φ is almost everywhere in Ω odd with respect to x_1 and that ψ is almost everywhere even in Ω with respect to x_1. Then*

$$\int_\Omega \varphi \cdot \overline{\psi} = 0.$$

PROOF. First note that by the Cauchy–Schwartz inequality $\varphi \cdot \overline{\psi} \in L^1(\Omega)$. Furthermore one has

$$\varphi(x_1, x_2, \dots, x_d) \cdot \overline{\psi}(x_1, x_2, \dots, x_d) = -\varphi(-x_1, x_2, \dots, x_d) \cdot \overline{\psi}(-x_1, x_2, \dots, x_d)$$

for almost every $x \in \Omega$ and hence $u = \varphi \cdot \overline{\psi}$ is almost everywhere in Ω odd with respect to x_1. The integral over an almost everywhere odd function $u \in L^1(\Omega)$ is

$$\begin{aligned}\int_\Omega u(x_1, x_2, \dots, x_d)dx &= \int_{\Omega_+} u(x_1, x_2, \dots, x_d)dx + \int_{\Omega_-} u(x_1, x_2, \dots, x_d)dx \\ &= \int_{\Omega_+} u(x_1, x_2, \dots, x_d)dx - \int_{\Omega_-} u(-x_1, x_2, \dots, x_d)dx \\ &= 0.\end{aligned}$$

□

From Lemma 5.19 one deduces that for any $v^{odd} \in H_0^1(\Omega)^{odd}$ and $u^{even} \in H_0^1(\Omega)^{even}$

$$\int_\Omega \langle Dv^{odd}, Du^{even}\rangle_{\mathbb{C}^d} = \sum_{j=1}^{d} \int_\Omega \langle (Dv^{odd})_j, (Du^{even})_j\rangle_{\mathbb{C}} = 0$$

because the addend with $j = 1$ is the product of an almost everywhere even and an almost everywhere odd functions, and the rest of the summands is the product of almost everywhere odd and almost everywhere even functions. Together with (74) this gives that one has even an orthogonal decomposition

$$H_0^1(\Omega) = H_0^1(\Omega)^{even} \oplus H_0^1(\Omega)^{odd} \tag{75}$$

of the Hilbert space $H_0^1(\Omega)$. This permits to apply methods from the theory of block operator matrices. Define the closed subspaces of $\operatorname{Ran} D$

$$\mathcal{H}_1 = DH_0^1(\Omega)^{even} \quad \text{and} \quad \mathcal{H}_2 = DH_0^1(\Omega)^{odd}. \tag{76}$$

From (75) and (76) it follows directly that

$$\operatorname{Ran} D = \mathcal{H}_1 \oplus \mathcal{H}_2 \tag{77}$$

Denote by P_1 the orthogonal projector in the Hilbert space $\operatorname{Ran} D$ onto the closed subspace $\mathcal{H}_1$ and accordingly by P_2 the orthogonal projector onto $\mathcal{H}_2$. The form $\mathfrak{a}$ given by

$$\mathfrak{a}[\psi,\varphi] = \langle \psi, M_A\varphi\rangle_{L^2(\Omega)^d}, \quad \psi,\varphi \in \operatorname{Ran} D$$

defines uniquely the bounded operator QM_AQ^*. One considers now the block operator matrix representation

$$QM_AQ^* = \begin{bmatrix} P_1QM_AQ^*P_1 & P_1QM_AQ^*P_2 \\ P_2QM_AQ^*P_1 & P_2QM_AQ^*P_2 \end{bmatrix}$$

and calculates each block in terms of sesquilinear forms. The operator $P_2QM_AQ^*P_2$ as an operator in $\mathcal{H}_2 = DH_0^1(\Omega)^{odd}$ is defined by the form $\mathfrak{a}_{2,2}$ given by

$$\mathfrak{a}_{2,2}[\psi,\varphi] = \langle \psi, M_A\varphi\rangle_{L^2(\Omega)^d}, \quad \text{where } \psi,\varphi \in \mathcal{H}_2,$$

compare for example [58, Chapter V §2.1]. One has

$$\langle \psi, M_A\varphi\rangle_{L^2(\Omega)^d} = \sum_{j=1}^d \int_\Omega \langle (Dv)_j, \operatorname{sign}(x_1)(Du)_j\rangle_{\mathbb{C}},$$

for $\psi = Dv$, $\varphi = Du$, where $u, v \in H_0^1(\Omega)^{odd}$. One observes that the summands

$$\langle (Dv)_j, \operatorname{sign}(x_1)(Du)_j\rangle_{\mathbb{C}}$$

are all odd with respect to x_1, because for $j = 1$ one has a product of the even function $(Dv)_1$, the odd function $\operatorname{sign}(x_1)$ and the odd function $(Du)_1$ which gives an odd function, and for $1 < j \leq d$ one has a product of three odd functions which is again odd with respect to x_1. By Lemma 5.19 the integrals vanish and one has

$$\mathfrak{a}_{2,2}[\psi,\varphi] = 0, \quad \text{for any } \psi,\varphi \in \mathcal{H}_2,$$

and therefore $P_2QM_AQ^*P_2 = 0$. The operator $P_1QM_AQ^*P_1$ is defined uniquely by the form $\mathfrak{a}_{1,1}$ given by

$$\mathfrak{a}_{1,1}[\psi,\varphi] = \langle \psi, M_A\varphi\rangle_{L^2(\Omega)^d}, \quad \psi,\varphi \in \mathcal{H}_1,$$

and again one has

$$\langle \psi, M_A\varphi\rangle_{L^2(\Omega)^d} = \sum_{j=1}^d \int_\Omega \langle (Dv)_j, \operatorname{sign}(x_1)(Du)_j\rangle_{\mathbb{C}},$$

for $\psi = Dv$, $\varphi = Du$ with $u, v \in H_0^1(\Omega)^{even}$. Now, the first summand is the product of the three odd functions $(Dv)_1$, $\operatorname{sign}(x_1)$ and $(Du)_1$ and therefore odd with respect to x_1. For $1 < j \leq d$ one has the product of the even function $(Dv)_j$, the odd function $\operatorname{sign}(x_1)$ and the even function $(Du)_j$ which is odd. Hence the integral vanishes identically and

$$\mathfrak{a}_{1,1}[\psi,\varphi] = 0, \quad \text{for any } \psi,\varphi \in \mathcal{H}_1,$$

and consequently also $P_1QM_AQ^*P_1 = 0$. Since the operator QM_AQ^* is self–adjoint it is sufficient to consider only one of the off–diagonal blocks, since the off–diagonal operators are adjoint to each other. Note that the operator $P_1QM_AQ^*P_2$ is a bounded operator from $\mathcal{H}_2 = DH_0^1(\Omega)^{odd}$ to $\mathcal{H}_1 = DH_0^1(\Omega)^{even}$. As such it is uniquely defined by the sesquilinear form $\mathfrak{a}_{2,1}$ in the Hilbert spaces $\mathcal{H}_1 \times \mathcal{H}_2$ which is defined by

$$\mathfrak{a}_{2,1}[\psi,\varphi] = \langle \psi, M_A\varphi\rangle_{L^2(\Omega)^d}, \quad \text{where } \psi \in \mathcal{H}_1 \quad \text{and } \varphi \in \mathcal{H}_2,$$

compare for example [58, Chapter V §2.1].

LEMMA 5.20. *Let $v \in H_0^1(\Omega)^{odd}$. Then $v \in H_0^1(\Omega_+) \oplus H_0^1(\Omega_-)$ and*

$$M_A D v = D \operatorname{sign}(x_1) v.$$

PROOF. The Hilbert space $H_0^1(\Omega_+) \oplus H_0^1(\Omega_-)$ is a closed subspace of $H_0^1(\Omega)$ and therefore the gradient operator

$$D_0 \colon H_0^1(\Omega_+) \oplus H_0^1(\Omega_-) \to L^2(\Omega)^d, \quad u \mapsto \operatorname{grad} u$$

is the restriction of the gradient operator D discussed in Section 5.1. A function $v \in H_0^1(\Omega)^{odd}$ has vanishing trace for $x_1 = 0$ because functions in $C_0^\infty(\Omega)$ that are odd with respect to x_1 have trace zero for $x_1 = 0$. Denote by $C_0^\infty(\Omega)^{odd}$ the space of functions in $C_0^\infty(\Omega)$ which are odd with respect to x_1 and by $C_0^\infty(\Omega)^{even}$ the space of functions in $C_0^\infty(\Omega)$ which are even with respect to x_1. One obtains with respect to the scalar product $\langle \cdot, \cdot \rangle_D$

$$C_0^\infty = C_0^\infty(\Omega)^{odd} \oplus C_0^\infty(\Omega)^{even},$$

and consequently $C_0^\infty(\Omega)^{odd} \subset H_0^1(\Omega)^{odd}$ is dense as well as $C_0^\infty(\Omega)^{even} \subset H_0^1(\Omega)^{even}$. Since the trace operator is bounded as an operator defined on $H_0^1(\Omega)$ the claim follows by continuous continuation from $C_0^\infty(\Omega)^{odd}$ to $H_0^1(\Omega)^{odd}$. As the trace of $v \in H_0^1(\Omega)^{odd}$ along the common boundary of Ω_+ and Ω_- is zero it follows by [76, Theorem 4.13] applied to Lipschitz domains that $v \in H_0^1(\Omega_+) \oplus H_0^1(\Omega_-)$. Note that the gradient D_0 in $H_0^1(\Omega_+) \oplus H_0^1(\Omega_-)$ acts on both parts separately and hence commutes with

$$A(x) = \operatorname{sign}(x_1)\mathbb{1} = \begin{cases} +\mathbb{1}, & \text{for } x \in \Omega_+, \\ -\mathbb{1}, & \text{for } x \in \Omega_-. \end{cases}$$

Consequently

$$M_A D v = M_A D_0 v = D_0 \operatorname{sign}(x_1) v = D \operatorname{sign}(x_1) v.$$

□

Note that $\operatorname{sign}(x_1) v \in H_0^1(\Omega)^{even}$ and hence Lemma 5.20 delivers that $M_A Q^* \varphi \in \mathcal{H}_2$, for $\varphi \in \mathcal{H}_1$. Therefore $P_2 Q M_A Q^* P_1$ acts just by multiplication

$$P_2 Q M_A Q^* P_1 \varphi = M_A \varphi, \quad \varphi \in \mathcal{H}_1.$$

In addition, $P_2 Q M_A Q^* P_1$ is a partial isometry between the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, because

$$\langle P_2 Q M_A Q^* P_1 \psi, P_2 Q M_A Q^* P_1 \varphi \rangle_{\mathcal{H}_2} = \langle M_A \psi, M_A \varphi \rangle_{L^2(\Omega)^d} = \langle \psi, \varphi \rangle_{\mathcal{H}_1},$$

for $\psi, \varphi \in \mathcal{H}_1$, where one used that $A(x)^2 = \mathbb{1}$ for all $x \in \Omega$.

LEMMA 5.21. *Let*

$$M = \begin{bmatrix} 0 & B^* \\ B & 0 \end{bmatrix}$$

be a block matrix operator in the separable Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, where

$$B \colon \mathcal{H}_2 \to \mathcal{H}_1$$

is a partial isometry between Hilbert spaces. Then

$$\{-1, 1\} \subset \sigma(M) \subset \{-1, 0, 1\}$$

and $0 \notin \sigma(M)$ if and only if B is surjective.

Now one can apply the above elementary lemma to the operator QM_AQ^* which delivers immediately Proposition 5.17. $\square$

PROOF OF LEMMA 5.21. Let $\{\phi_k\}_{k\in\mathbb{N}}$ be a complete orthonormal basis of $\mathcal{H}_2$. Then $\{B\phi_k\}_{k\in\mathbb{N}}$ is a complete orthonormal basis of the closed subspace $\operatorname{Ran} B \subset \mathcal{H}_1$. Denote furthermore by R the orthogonal projector in $\mathcal{H}_1$ onto $(\operatorname{Ran} B)^\perp$ and by $R^\perp = \mathbb{1} - R$ the complementary projector. The restricted block matrix operator $\widetilde{M}$ has the block matrix representation

$$\widetilde{M} = \begin{bmatrix} 0 & U^* \\ U & 0 \end{bmatrix}$$

with respect to $\operatorname{Ran} R^\perp \oplus \mathcal{H}_2$, where $U\colon \mathcal{H}_2 \to \operatorname{Ran} R^\perp$ is unitary. On the space spanned by the basis $\{B\phi_k, \phi_k\}$ the operator $\widetilde{M}$ acts simply as the matrix

$$\widetilde{M_k} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

which has the eigenvalues $+1$ and -1. The operator $\widetilde{M}$ can be written just as a direct sum of such operators $\widetilde{M_k}$ and consequently $\sigma(\widetilde{M}) = \{-1, +1\} \subset \sigma(M)$. Zero is not in the spectrum of M if and only if $\operatorname{Ran} B = \mathcal{H}_1$. For $\operatorname{Ran} B \subsetneq \mathcal{H}_1$ one has $\sigma(M) = \{-1, 0+1\}$. $\square$

REMARK 5.22. *The starting point for the formulation of Proposition 5.17 has been the following observation in dimension* $d = 1$. *Consider* $\Omega = \left(\frac{\pi}{2}, \frac{\pi}{2}\right)$ *and set*

$$\Omega_+ = (0, \pi/2) \quad \textit{and} \quad \Omega_- = (-\pi/2, 0).$$

The eigenfunctions of the Dirichlet Laplacian form a complete orthogonal basis of the Hilbert space $H_0^1(\Omega)$. *They are*

$$\phi_n = \begin{cases} \cos(nx), & \textit{for } n = 2m-1, \\ \sin(nx), & \textit{for } n = 2m \quad \textit{with } m \in \mathbb{N}, \end{cases}$$

and the corresponding eigenvalue to ϕ_n *is* n^2, $n \in \mathbb{N}$. *Note that the space* $H_0^1(\Omega)^{odd}$ *is spanned by the* $\sin$*–type–functions and the space* $H_0^1(\Omega)^{even}$ *by the* $\cos$*–type–functions. Furthermore one observes that the functions* $\cos(n\,\cdot)$, *where* $n = 2m-1$ *are the eigenfunctions of the Laplace operator with Dirichlet boundary conditions at* $\pi/2$ *and Neumann boundary conditions imposed at the point* 0. *In contrast the functions* $\sin(n\,\cdot)$ *with* $n = 2m$ *are the eigenfunctions of the Laplace operator with Dirichlet boundary conditions at both endpoints* $\pi/2$ *and* 0. *A relationship between certain sign–indefinite operators and sign–definite operators has been observed also in Remark 4.13 in Chapter 4, when investigating the limit behaviour of a sign–indefinite operator.*

EXAMPLE 5.23. *Consider as in Example 5.16*

$$A(x) = \operatorname{sign}(x_1) \cdot \mathbb{1}, \quad \textit{where } x = (x_1, x_2) \in \Omega = (-a, a) \times (0, 1).$$

Applying Proposition 5.17 and using the information from Example 5.16 gives for this case

$$\sigma(QM_AQ^*) = \{-1, 0, +1\}.$$

I would like to close this Chapter by stating two conjectures. The case discussed in Proposition 5.12 seems to me exemplary for a class of coefficients $A(\cdot)$. This is made precise in the following

CONJECTURE 5.24. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and let $A(\cdot), A(\cdot)^{-1} \in L^\infty(\Omega)^{d\times d}$. If the Lebesgue measure of the set*

$$S_{ind}(A) = \{x \in \Omega \mid \operatorname{sign} A(x) \textit{ is indefinite}\}$$

is larger than zero, then QM_AQ^* has no gap in the spectrum. This means there is no $\lambda \in \mathbb{R}$ such that $QM_AQ^* - \lambda = QM_{A-\lambda}Q^*$ is boundedly invertible and sign–indefinite.

Eventually, there is at least a small class of examples with QM_AQ^* invertible, and in this case the coefficient $A(\cdot)$ is piecewise elliptic. I suspect that the arguments used in the proof can be localized in order to generalize Proposition 5.17. However at present I am not able to perform this, nevertheless I would like to formulate the following

CONJECTURE 5.25. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $A(\cdot), A(\cdot)^{-1} \in L^\infty(\Omega)^{d\times d}$. Assume that there are non–empty open sets $\Omega_\pm \subset \Omega$ such that*

$$\Omega_- \cap \Omega_+ = \emptyset, \qquad \overline{\Omega_-} \cup \overline{\Omega_+} = \overline{\Omega},$$

and the matrix $\pm A(x)$ is positive definite for almost every $x \in \Omega_\pm$. Then QM_AQ^* has a gap in the spectrum, which means there are $\lambda \in \mathbb{R}$ such that $QM_AQ^* - \lambda = QM_{A-\lambda}Q^*$ is boundedly invertible and sign–indefinite.

The absence of a general criterion for dimension $d \geq 2$ identifying invertible and indefinite operators QM_AQ^* is disappointing and dissatisfying. Nevertheless, the operator QM_AQ^* is one key for the understanding of the operator theory of indefinite differential operators of the type D^*M_AD, since it arises naturally when considering operators in the div–grad–form and the associated quadratic forms.

CHAPTER 6

Eigenvalue asymptotics and variational methods

Consider the sign–indefinite self–adjoint operator $\mathcal{L}$ constructed in Theorem 5.4 of the previous chapter and recall that $\mathcal{L}$ has purely discrete spectrum. This chapter is devoted to the study of the asymptotic behaviour of the eigenvalues of $\mathcal{L}$. I am conjecturing that the asymptotic distribution of the eigenvalues satisfies a generalized Weyl law. The main result is that in dimension $d = 1$ the conjecture is indeed true, and in higher dimensions at least bounds on the asymptotic behaviour of the eigenvalues are obtained. The conjecture is based on the study of the one dimensional model problem which is elaborated in Proposition 4.21 of Chapter 4, where a generalized Weyl law for certain indefinite operators on metric graphs has been proven.

The study of the distribution of eigenvalues is inseparably linked to the name of H. Weyl. His study of the asymptotic behaviour of the eigenvalues of Dirichlet Laplacians on bounded domains, see [94], was motivated by the radiation problem, see also [6] for an overview of the history of the problem. The Dirichlet Laplacian is the unique self–adjoint operator associated with the symmetric form defined by $\langle \operatorname{grad} v, \operatorname{grad} u\rangle_{L^2(\Omega)^d}$, where $v, u \in H_0^1(\Omega) \subset L^2(\Omega)$, and it has only discrete spectrum. H. Weyl found out that on bounded domains the counting function of the Dirichlet Laplacian behaves asymptotically like

$$N^+(\lambda) \sim (2\pi)^{-d}\omega_d|\Omega|\lambda^{d/2}, \quad \lambda \to \infty,$$

where ω_d is the volume of the unit ball in $\mathbb{R}^d$ and $|\Omega|$ denotes the Lebesgue measure of $\Omega \subset \mathbb{R}^d$, where it is supposed that Ω is bounded. The Weyl law states in particular that the leading term of the counting function is asymptotically proportional to the volume of the domain Ω. The question of the asymptotic distribution of eigenvalue has been extended to elliptic differential operators on bounded domains, see for example [1], and even to generalized eigenvalue problems, see [17]. At present the counting functions of the eigenvalues of elliptic self–adjoint operators are well studied objects, see for example [57] and the references therein.

There are two main techniques which are used in the studies of eigenvalue asymptotics: the so called Tauberian method introduced by T. Carleman, see [23, 24], which in general requires several smoothness assumptions and the variational methods, which were used originally by H. Weyl. In the subsequent section a variational characterization of the eigenvalues of the operator $\mathcal{L}$ is given. The main results are formulated in Section 6.2. The proofs are are based on variational arguments and are given in Section 6.3.

6.1. Variational characterization of the eigenvalues

The eigenvalue problem for the self–adjoint operator $\mathcal{L}$, constructed in Theorem 5.4 of the previous chapter, consists in finding numbers $\lambda \neq 0$ and non–trivial $u = u(\lambda)$ to solve the equation $\mathcal{L}u = \lambda u$, where $u \in \operatorname{Dom}(\mathcal{L})$. Taking into account that the operator $\mathcal{L}$ is invertible and has pure point spectrum one concludes that the restriction

$$\mathcal{L}\mid_{\mathrm{Ker}(\mathcal{L}-\lambda)}\colon\ \mathrm{Ker}(\mathcal{L}-\lambda)\longrightarrow \mathrm{Ker}(\mathcal{L}-\lambda)$$

is an isomorphism between finite dimensional spaces, because the eigenspaces are invariant subspaces of $\mathcal{L}$. Therefore having a solution $u=u(\lambda)$ with $\lambda\neq 0$ of the original problem this is consequently also a solution (with the same multiplicity) of

$$\lambda^{-1}\mathcal{L}^2 u=\mathcal{L}u,\quad u\in\mathrm{Dom}(\mathcal{L}^2) \tag{78}$$

and vice versa. Following the guideline of M. Š. Birman and M. Z. Solomyak, see [17] and the references therein, one investigates instead of unbounded operators their resolvents and particularly their inverses.

Denote by

$$0<\lambda_1^+\leq\lambda_2^+\leq\ldots\leq\lambda_j^+\leq\ldots,\quad j\in\mathbb{N},$$

and by

$$0>-\lambda_1^-\geq-\lambda_2^-\geq\ldots\geq-\lambda_j^-\geq\ldots,\quad j\in\mathbb{N},$$

the positive and negative eigenvalues of $\mathcal{L}$ enumerated in the increasing and decreasing order, respectively, counting their multiplicities.

PROPOSITION 6.1. *Let $\mathcal{L}$ be the operator referred to in Theorem 5.4. Then the following variational formulae hold*

$$\left(\lambda_{j+1}^{\pm}\right)^{-1}=\min_{\substack{\mathfrak{H}\subset\mathrm{Dom}(\mathcal{L})\\ \mathrm{codim}\mathfrak{H}\leq j}}\ \max_{\substack{u\in\mathfrak{H}\\ u\neq 0}}\pm\frac{\langle u,\mathcal{L}u\rangle}{\langle\mathcal{L}u,\mathcal{L}u\rangle},\quad j\in\mathbb{N}_0. \tag{79}$$

REMARK 6.2.

(1) The variational characterization of the eigenvalues given in Proposition 6.1 remains valid for any self–adjoint operator with compact inverse, semi–boundedness is not necessary.

(2) The quotient given in (79) *can be interpreted equivalently as the generalized Rayleigh quotient of the linear operator pencil $\mathcal{P}(\mu)=\mu\mathcal{L}^2-\mathcal{L}$, $\mu\in\mathbb{R}$.*

(3) Observe that on the left hand side of (78) *one has a positive forth order operator and on the right hand side an indefinite second order operator. This is a situation that is in some particular cases comparable to the one studied by M. Š. Birman and M. Z. Solomyak in the article [17]. One difference is that the operator $\mathcal{L}^2$ on the left hand side is not elliptic in the classical sense.*

PROOF. As $\mathcal{L}$ is a self-adjoint boundedly invertible operator, its domain $\mathrm{Dom}(\mathcal{L})$ equipped with the inner product defined by

$$\langle v,u\rangle_{\mathcal{L}}=\langle\mathcal{L}v,\mathcal{L}u\rangle_{L^2(\Omega)}$$

is a Hilbert space, denoted by $\mathcal{H}_{\mathcal{L}}$. One considers the operators

$$\mathcal{L}_1\colon\mathcal{H}_{\mathcal{L}}\longrightarrow L^2(\Omega),\quad u\mapsto\mathcal{L}u$$

and

$$\mathcal{L}_2\colon\mathcal{H}_{\mathcal{L}}\supset\mathrm{Dom}(\mathcal{L}^2)\longrightarrow\mathrm{Dom}(\mathcal{L})=\mathcal{H}_{\mathcal{L}},\quad u\mapsto\mathcal{L}u.$$

The definition of the inner product $\langle\cdot,\cdot\rangle_{\mathcal{L}}$ implies that the operator $\mathcal{L}_1$ is isometric. Since its range agrees with $L^2(\Omega)$, it is unitary. The operator $\mathcal{L}_2$ is a closed densely defined unbounded operator. From

$$\langle v, \mathcal{L}_2 u\rangle_{\mathcal{L}} = \langle \mathcal{L}v, \mathcal{L}^2 u\rangle_{L^2(\Omega)} = \langle \mathcal{L}^2 v, \mathcal{L}u\rangle_{L^2(\Omega)} = \langle \mathcal{L}_2 v, u\rangle_{\mathcal{L}}, \quad u, v \in \mathrm{Dom}(\mathcal{L}^2),$$

it follows that $\mathcal{L}_2$ is symmetric. Since $\mathcal{L}_2$ is surjective, it is also self-adjoint, see for example [83, Section X.1]. Both $\mathcal{L}_1$ and $\mathcal{L}_2$ act as $\mathcal{L}$ but in different spaces and have different domains. The relation between them is summarized in the following commutative diagram,

$$\begin{array}{ccc} \mathcal{H}_{\mathcal{L}} \supset \mathrm{Dom}(\mathcal{L}^2) & \xrightarrow{\mathcal{L}_2} & \mathrm{Dom}(\mathcal{L}) \subset \mathcal{H}_{\mathcal{L}} \\ \Big\downarrow \mathcal{L}_1|_{\mathrm{Dom}(\mathcal{L}^2)} & & \Big\downarrow \mathcal{L}_1 \\ L^2(\Omega) \supset \mathrm{Dom}(\mathcal{L}) & \xrightarrow{\mathcal{L}} & L^2(\Omega), \end{array}$$

from which one reads out the equality

$$\mathcal{L}_2^{-1} = \mathcal{L}_1^{-1}\mathcal{L}^{-1}\mathcal{L}_1.$$

Since $\mathcal{L}_1$ is unitary and the operator $\mathcal{L}^{-1}$ is compact by Theorem 5.4, the inverse of the operator $\mathcal{L}_2$ is compact as well. Hence the eigenvalues of $\mathcal{L}_2$ can be determined by means of the $\min$–$\max$–principle using the Rayleigh quotient

$$\rho[u] := \frac{\langle u, \mathcal{L}_2^{-1}u\rangle_{\mathcal{L}}}{\langle u, u\rangle_{\mathcal{L}}} = \frac{\langle u, \mathcal{L}u\rangle}{\langle \mathcal{L}u, \mathcal{L}u\rangle}, \quad u \in \mathrm{Dom}(\mathcal{L}), \tag{80}$$

see for example [40]. Observing that the operators $\mathcal{L}$ and $\mathcal{L}_2$ have the same eigenvalues (counted with multiplicities) and the same eigenvectors, completes the proof of the proposition. □

6.2. The asymptotic behaviour of the eigenvalues

Let $N^{\pm}$ be the counting functions for the positive and the negative eigenvalues of the operator $\mathcal{L}$, which are defined by

$$N^{\pm}(\lambda) = \#\{\lambda_j^{\pm} \le \lambda\}.$$

Recall that λ_j^+ and $-\lambda_j^-$, $j \in \mathbb{N}$ denote the positive and negative eigenvalues of $\mathcal{L}$ enumerated in the increasing and decreasing order, respectively, counting their multiplicities. The variational characterization of the eigenvalues delivers the subsequent estimate on the order of the counting functions.

THEOREM 6.3. *There are non–negative constants $C^{\pm} \ge 0$, such that*

$$N^{\pm}(\lambda) \le C^{\pm}\,\lambda^{d/2}$$

and

$$C^{\pm} \le \|(QM_AQ^*)_{\pm}^{-1}\|(2\pi)^{-d}\omega_d|\Omega|,$$

where $(QM_AQ^*)_{\pm}^{-1}$ denotes the positive, respectively the negative part of $(QM_AQ^*)^{-1}$.

The proof is postponed to Section 6.3. The above theorem and Proposition 4.21 in Chapter 4 give rise to the following conjecture on the asymptotic distribution of the eigenvalues.

CONJECTURE 6.4. *The eigenvalue counting functions of the operator $\mathcal{L}$ satisfy a generalized Weyl law, that is*

$$N^{\pm}(\lambda) \sim \frac{(2\pi)^{-d}}{d}\omega^{\pm}\lambda^{d/2}, \quad \textit{for } \lambda \to \infty,$$

where

$$\omega^{\pm} = \int_{\Omega}\int_{|\xi|=1} \left(\langle \xi, A(x)\xi\rangle_{\mathbb{C}^d}\right)_{\pm}^{-d/2} d\sigma(\xi)dx,$$

with $(t)_{\pm} := (|t| \pm t)/2$ and σ the Lebesgue measure on the unit sphere in $\mathbb{R}^d$.

The notion $\sim$ is explained in (89) and the following.

REMARK 6.5. *Assume that there are non–empty open sets $\Omega_{\pm} \subset \Omega$ such that*

$$\Omega_- \cap \Omega_+ = \emptyset, \qquad \overline{\Omega_-} \cup \overline{\Omega_+} = \overline{\Omega},$$

and that the matrix $\pm A(x)$ is positive definite for almost all $x \in \Omega_{\pm}$. Suppose furthermore that QM_AQ^* is boundedly invertible. Then Conjecture 6.4 can be re–formulated as

$$N^{\pm}(\lambda) \sim N_{\Omega_{\pm}}(\lambda), \quad \textit{for } \lambda \to \infty,$$

where $N_{\Omega_{\pm}}(\lambda)$ are the eigenvalue counting functions of the elliptic differential operators $\pm\mathcal{L}_{\pm}$. The operators $\mathcal{L}_{\pm}$ are the unique operators that are associated with the closed symmetric semi–bounded sesquilinear forms $\mathfrak{l}_{\pm}$ which are defined by

$$\mathfrak{l}_{\pm}[v,u] = \langle \operatorname{grad} v, A(\cdot)\operatorname{grad} u\rangle_{L^2(\Omega_{\pm})^d}, \qquad v,u \in H_0^1(\Omega_{\pm}) \subset L^2(\Omega_{\pm}).$$

In particular the conjecture states that asymptotically the spectrum of the operator $\mathcal{L}$ resembles the spectrum of the direct sum of a positive definite and a negative definite operator. In dimension $d = 1$ the conjecture is indeed true.

THEOREM 6.6. *Let Ω be a bounded interval. Suppose that $A(\cdot), A(\cdot)^{-1} \in L^{\infty}(\Omega;\mathbb{R})$ and that*

$$\int_{\Omega} A(x)^{-1}dx \neq 0.$$

Then the eigenvalue counting functions of the operator $\mathcal{L}$ constructed in Theorem 5.4 have the asymptotics

$$N^{\pm}(\lambda) \sim \frac{1}{\pi}\omega^{\pm}\lambda^{1/2}, \quad \lambda \to \infty, \tag{81}$$

where

$$\omega^{\pm} = \int_{\Omega} (A(x))_{\pm}^{-1/2}\, dx.$$

The asymptotic formulae given in equation (81) agree with the more general formulae for the asymptotic behaviour of the eigenvalues of sign-indefinite Sturm-Liouville operators. The most general result known to me in this context is due to P. A. Binding and H. Volkmer, see [15], where also further references on eigenvalue problems for Sturm-Liouville operators involving sign–indefinite coefficients are given. Their and also previous results, like the one of F. V. Atkinson and A. B. Mingarelli, see [8], are valid under weaker assumptions on the coefficient $A(\cdot)$, than those needed here. The proof of P. A. Binding and H. Volkmer takes advantage of the oscillation of the eigenfunctions and the Prüfer angle, whereas the proof of Theorem 6.6 given here is based on variational arguments and perturbation theory.

EXAMPLE 6.7. *Consider as in Example 5.6 an open interval $\Omega = (a, b)$ and a measurable subset $\Omega_+ \subset \Omega$. Set $\Omega_- = \Omega \setminus \Omega_+$ and consider*

$$A(x) = \begin{cases} +1, & x \in \Omega_+, \\ -1, & x \in \Omega_-. \end{cases}$$

Assume that $|\Omega_-| \neq |\Omega_+|$. Hence the assumptions of Theorem 6.6 are satisfied and the coefficients in the counting functions are

$$\omega_+ = \frac{|\Omega_+|}{\pi} \quad \text{and} \quad \omega_- = \frac{|\Omega_-|}{\pi}.$$

I have not been able to prove Conjecture 6.4 in a more general situation. However one can show that in particular cases the conjectured formulae form lower bounds on the counting functions of $\mathcal{L}$.

THEOREM 6.8. *Let Ω be a bounded Lipschitz domain and Ω_+, Ω_- open sets such that*

$$\Omega_- \cap \Omega_+ = \emptyset \quad \text{and} \quad \overline{\Omega_-} \cup \overline{\Omega_+} = \overline{\Omega}.$$

Let $A_\pm(\cdot) \in C^\infty(\Omega_\pm)^{d\times d}$, where $\pm A_\pm(x)$ are Hermitian and positive for almost every $x \in \Omega_\pm$, with $A(\cdot), A^{-1}(\cdot) \in L^\infty(\Omega; \mathbb{C})^{d\times d}$. Consider

$$A(x) = \begin{cases} A_+(x), & x \in \Omega_+, \\ A_-(x), & x \in \Omega_- \end{cases}$$

and suppose that QM_AQ^* is boundedly invertible. Then $H_0^2(\Omega_+) \oplus H_0^2(\Omega_-) \subset \mathrm{Dom}(\mathcal{L})$ and

$$N_{\Omega_\pm}(\lambda) \lesssim N^\pm(\lambda), \quad \text{for } \lambda \to \infty,$$

where $N_{\Omega_\pm}$ are the counting functions introduced in Remark 6.5 and the notion $\lesssim$ is explained below in (89) *and the following.*

Note that under the assumptions of the above theorem the multiplication operators $\pm M_{A_\pm}$ in $L^2(\Omega_\pm)^d$ are strictly positive. Together with Theorem 6.3 one obtains that in the above situation the order of the counting functions is indeed $\lambda^{d/2}$.

REMARK 6.9. *The proof of Theorem 6.8 is based on the variational characterization of the eigenvalues of $\mathcal{L}$ and the comparison of the corresponding Rayleigh quotient to certain generalized eigenvalue problems which were studied by M. Š. Birman and M. Z. Solmyak in the article [17]. If in addition one was able to prove the inclusion*

$$\mathrm{Dom}(\mathcal{L}) \subset H^2(\Omega_+) \oplus H^2(\Omega_-)$$

and furthermore the inequality

$$\|u\|^2_{H^2(\Omega_+)} + \|u\|^2_{H^2(\Omega_-)} \leq C\|\mathcal{L}u\|^2, \quad \text{for } C > 0 \text{ and all } u \in \mathrm{Dom}(\mathcal{L}),$$

applying the above mentioned method would deliver the proof of the conjecture in a straightforward way for this particular case. This would be analogous to the proof of Proposition 6.13.

A case study. Let $\Omega = (0,b)\times(-a,a) \subset \mathbb{R}^2$ for $a,b>0$ and let $c_+, c_- > 0$ with $c_- \neq c_+$. Consider

$$A(x) = \begin{cases} +c_+ \cdot \mathbb{1}, & \text{for } x \in \Omega_+ = (0,b)\times(0,a), \\ -c_- \cdot \mathbb{1}, & \text{for } x \in \Omega_- = (0,b)\times(-a,0). \end{cases}$$

Then by Proposition 5.17 Theorem 5.4 applies and the spectrum of the operator $\mathcal{L}$ is discrete. Hence one can analyse the counting functions.

Assume for simplicity that $b=1$. Note that by separation of variables one has that any $\psi \in L^2(\Omega)$ can be represented by the Fourier series

$$\psi(x,y) = \sum_{n\in\mathbb{N}} \psi_n(x)\phi_n(y),$$

where $\phi_n(y) = \sin\left((\pi n)\, y\right)$ and

$$\psi_n(x) = \frac{\langle \psi(x,\cdot), \phi_n\rangle_{L^2([0,1],dy)}}{\|\phi_n\|^2_{L^2([0,1],dy)}}. \tag{82}$$

This Fourier series decomposition delivers the map

$$U_n \colon L^2(\Omega) \to L^2([-a,a],dx_n), \quad \psi \mapsto \psi_n,$$

the adjoint of which is the immersion

$$U_n^* \colon L^2([-a,a],dx_n) \to L^2(\Omega), \quad \psi_n \mapsto \psi_n \cdot \phi_n.$$

The map

$$U \colon L^2(\Omega) \to \bigoplus_{n\in\mathbb{N}} L^2([-a,a],dx_n), \quad \psi \mapsto \{\psi_n\}_{n\in\mathbb{N}}$$

is unitary and $U = \bigoplus_{n\in\mathbb{N}} U_n$. The operator $\mathcal{L}_U := UD^*M_ADU^*$ is the direct sum

$$\mathcal{L}_U = \bigoplus_{n\in\mathbb{N}} \mathcal{L}_n,$$

where $\mathcal{L}_n = U_n\mathcal{L}U_n^*$ are operators in $L^2([-a,a],dx_n)$. A direct calculation gives that for any $\psi \in \mathrm{Dom}(\mathcal{L})$

$$\mathcal{L}_n\psi_n = -\frac{d}{dx_n}A(\cdot)\frac{d}{dx_n}\psi_n + A(\cdot)(n\pi)^2\psi_n,$$

where $\psi_n = U_n\psi$ is given by (82) and with a slide abuse of notation the function $A(\cdot)$ is defined by

$$A(x_n) = \begin{cases} +c_+, & \text{for } x_n \geq 0, \\ -c_-, & \text{for } x_n < 0. \end{cases}$$

For $\psi \in \mathrm{Dom}(\mathcal{L})$ one has $\psi_n \in \mathrm{Dom}(\mathcal{L}_n)$, where

$$\mathrm{Dom}(\mathcal{L}_n) = \left\{\psi_n \in H_0^1([-a,a],dx_n) \mid A(\cdot)\tfrac{d}{dx_n}\psi_n \in H^1([-a,a],dx_n)\right\}.$$

The operator $\mathcal{L}_n$ is self–adjoint and hence the direct sum $\mathcal{L}_U$ is self–adjoint too, see for example [93, Theorem 18.2]. Furthermore one has

$$\sigma(\mathcal{L}) = \sigma(\mathcal{L}_U) = \overline{\bigcup_{n\in\mathbb{N}} \sigma(\mathcal{L}_n)},$$

see also [93, Theorem 18.2]. Therefore it is sufficient to analyse the spectrum of each $\mathcal{L}_n$. Note that the spectrum of $\mathcal{L}_n$ is purely discrete.

An *Ansatz* for an eigenfunction of $\mathcal{L}_n$ to a positive eigenvalue $\lambda > c_+(n\pi)^2$ is given by

$$\varphi_n(x_n,\lambda) = \begin{cases} \alpha_n(\lambda)\sin\left(\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}(a - x_n)\right), & x_n \in (0,a], \\ \beta_n(\lambda)\sinh\left(\sqrt{\frac{\lambda}{c_-} + \pi^2 n^2}(a + x_n)\right), & x_n \in [-a,0), \end{cases}$$

for appropriate coefficients $\alpha_n(\lambda)$ and $\beta_n(\lambda)$. The function $\varphi_n(\cdot,\lambda)$ is an eigenfunction of $\mathcal{L}_n$ to the eigenvalue λ if and only if $\varphi_n(\cdot,\lambda) \in \operatorname{Dom}(\mathcal{L}_n)$ which is the case if and only if the matching conditions

$$\lim_{\epsilon\to 0+} \varphi_n(\epsilon,\lambda) = \lim_{\epsilon\to 0-} \varphi_n(\epsilon,\lambda)$$

and

$$\lim_{\epsilon\to 0+} c_+ \frac{d}{dx_n}\varphi_n(\epsilon,\lambda) = -c_- \lim_{\epsilon\to 0-} \frac{d}{dx_n}\varphi_n(\epsilon,\lambda)$$

are satisfied. This is encoded in the equation

$$\begin{bmatrix} \sin\left(a\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}\right) & \sinh\left(a\sqrt{\frac{\lambda}{c_-} + \pi^2 n^2}\right) \\ c_+\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}\cos\left(a\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}\right) & c_-\sqrt{\frac{\lambda}{c_-} + \pi^2 n^2}\cosh\left(a\sqrt{\frac{\lambda}{c_-} + \pi^2 n^2}\right) \end{bmatrix} \begin{bmatrix} \alpha_n(\lambda) \\ \beta_n(\lambda) \end{bmatrix} = 0.$$

It follows that there are suitable coefficients $\alpha_n(\lambda)$ and $\beta_n(\lambda)$ if and only if $\lambda > c_+(n\pi)^2$ is a solution of the secular equation

$$\tan\left(a\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}\right) = \frac{c_+\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}}{c_-\sqrt{\frac{\lambda}{c_-} + \pi^2 n^2}} \tanh\left(a\sqrt{\frac{\lambda}{c_-} + \pi^2 n^2}\right).$$

Note that the function on the right hand side is strictly increasing for $\lambda > c_+(n\pi)^2$, whereas the the function on the left hand side is periodic. Denote by λ_m^n for $m \geq 1$ the positive eigenvalues of $\mathcal{L}_n$ with $\lambda_m^n > c_+\pi^2 n^2$ counting their multiplicities,

$$c_+\pi^2 n^2 < \lambda_1^n \leq \lambda_2^n \leq \lambda_3^n \leq \dots$$

Define the counting function for eigenvalues λ_m^n with $\lambda > c_+\pi^2 n^2$ by

$$N_1^+(\lambda) = \#\{\lambda_m^n \mid c_+\pi^2 n^2 < \lambda_m^n \leq \lambda\}.$$

Denote by μ_m^n and ν_m^n the zeros of

$$\sin\left(a\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}\right) = 0 \quad \text{and} \quad \cos\left(a\sqrt{\frac{\lambda}{c_+} - \pi^2 n^2}\right) = 0$$

with $\mu_m^n > c_+\pi^2n^2$ and $\nu_m^n > c_+\pi^2n^2$, respectively. Using the intermediate value theorem one can show that

$$\nu_m^n \leq \lambda_m^n \leq \mu_m^n, \quad \text{for } m,n \in \mathbb{N}. \tag{83}$$

Note that μ_m^n for $n,m \in \mathbb{N}$ are exactly the eigenvalues of the Dirichlet Laplacian multiplied with c_+ on $L^2(\Omega_+)$ with $\Omega_+ = (0,1) \times (0,a)$. The numbers ν_m^n for $n,m \in \mathbb{N}$ are exactly the eigenvalues of the Laplacian on $L^2(\Omega_+)$ multiplied by c_+ with Dirichlet boundary conditions imposed at the outer boundary $\partial\Omega \cap \partial\Omega_+$ and Neumann boundary conditions at the inner boundary $\partial\Omega_+ \setminus \partial\Omega$. These two operators satisfy the classical Weyl law and from (83) it follows that

$$N_1^+(\lambda) \sim N_{\Omega_+}(\lambda), \quad \text{for } \lambda \to \infty.$$

For the counting function of the negative eigenvalues with $\lambda_n < c_-\pi^2n^2$ one obtains the analogous result.

For $-c_-(n\pi)^2 < \lambda < c_+(n\pi)^2$ one has the Ansatz

$$\psi_n(x_n,\lambda) = \begin{cases} \alpha_n(\lambda)\sinh\left(\sqrt{\frac{\lambda}{c_+} - \pi^2n^2}(a - x_n)\right), & x_n \in (0,a], \\ \beta_n(\lambda)\sinh\left(\sqrt{\frac{\lambda}{c_-} + \pi^2n^2}(a + x_n)\right), & x_n \in [-a,0). \end{cases}$$

For $c_+ > c_-$ there is at most one eigenvalue $0 < \lambda_0^n < c_+(n\pi)^2$ which is the solution of

$$\tanh\left(a\sqrt{\pi^2n^2 - \frac{\lambda}{c_+}}\right) = \frac{c_+\sqrt{\pi^2n^2 - \frac{\lambda}{c_+}}}{c_-\sqrt{\frac{\lambda}{c_-} + \pi^2n^2}} \tanh\left(a\sqrt{\frac{\lambda}{c_-} + \pi^2n^2}\right). \tag{84}$$

For $c_+ = c_-$ the operator QM_AQ^* is not boundedly invertible anymore, compare Example 5.16. However one can analyse the operator $\mathcal{L}' = \overline{D^*M_AD}$ using a separation of variables. In this case (84) has the unique solution zero for any $n \in \mathbb{N}$. For $c_+ \neq c_-$ I was not able to clarify the distribution of these *exceptional eigenvalues*. A better understanding of the distribution of the exceptional eigenvalues would deliver information on lower order terms of the eigenvalue counting function. I suspect that there is a relation between these exceptional eigenvalues of $\mathcal{L}$ and the eigenvalue $\frac{c_+ - c_-}{2}$ of QM_AQ^* lying between the spectral points c_+ and $-c_-$, compare Example 5.23.

However, in this concrete example one can show that for $c_+ \neq c_-$ the conjecture on the leading term of the eigenvalue counting function is indeed true. The asymptotic inequalities $N_{\Omega_\pm}(\lambda) \lesssim N^\pm(\lambda)$, for $\lambda \to \infty$ follow from Theorem 6.8 as well as from the above calculation. Here, the inequality $N^\pm(\lambda) \sim N_{\Omega_\pm}(\lambda)$, for $\lambda \to \infty$ is derived by considering the difference

$$(QM_AQ^*)^{-1} - QM_{A^{-1}}Q^*.$$

In the following it is shown that this difference is small in a certain sense, such that the leading term for the counting functions of the compact operators

$$D^{-1}(QM_AQ^*)^{-1}(D^*)^{-1} \quad \text{and} \quad D^{-1}QM_{A^{-1}}Q^*(D^*)^{-1}$$

are the same. Applying Proposition 6.13 below to the operator $QM_{A^{-1}}Q^*$ delivers the claim.

Note that for $c_+ = c_-$ Example 5.16 together with the proof of Proposition 5.17 provide the complete spectral resolution for the operator QM_AQ^*, and by a shift one obtains the same also for the case $c_+ \neq c_-$. More precisely, the proof of Proposition 5.17 exhibits that $-c_-$

and c_+ are isolated eigenvalues and that the only further possible point in the spectrum is zero. Example 5.16 shows that here, in the case of a rectangle, zero is indeed an eigenvalue of QM_AQ^* if $c_+ = c_-$ holds. Furthermore the eigenfunctions to the eigenvalue zero are exactly given by the gradients of the solutions to the differential equation

$$-\operatorname{div} A(\cdot) \operatorname{grad} u = 0$$

referred to in Remark 5.15. The space of solutions to this equation is formed by the functions u_m, $m \in \mathbb{N}$, given in Example 5.16. So,

$$\sigma(QM_AQ^*) = \{c_+, \frac{c_+ - c_-}{2}, -c_-\},$$

and since QM_AQ^* is self-adjoint there are orthogonal projectors onto the corresponding eigenspaces. Denote by P_0 the orthogonal projector onto the eigenspace to the eigenvalue $\frac{c_+ - c_-}{2}$ which is exactly $\operatorname{span}\{Du_m \mid m \in \mathbb{N}\}$, and furthermore by P_+ and P_- the orthogonal projectors onto the eigenspaces of QM_AQ^* corresponding to the eigenvalues c_+ and $-c_-$, respectively. So, one has the representation

$$QM_AQ^* = c_+ P_+ + \frac{c_+ - c_-}{2} P_0 - c_- P_-,$$

and therefore

$$(QM_AQ^*)^{-1} = c_+^{-1} P_+ + \left(\frac{c_+ - c_-}{2}\right)^{-1} P_0 - c_-^{-1} P_-$$

along with

$$QM_{A^{-1}}Q^* = c_+^{-1} P_+ + \frac{c_+^{-1} - c_-^{-1}}{2} P_0 - c_-^{-1} P_-.$$

So,

$$(QM_AQ^*)^{-1} - QM_{A^{-1}}Q^* = c_0 P_0 \quad \text{with } c_0 = \left(\tfrac{c_+ - c_-}{2}\right)^{-1} - \tfrac{c_+^{-1} - c_-^{-1}}{2}.$$

Recall that P_0 is the direct sum of rank one projectors

(85) $$P_0 = \oplus_{m \in \mathbb{N}} P_m,$$

where P_m, $m \in \mathbb{N}$, is the orthogonal projector onto the one dimensional space $\operatorname{span}\{Du_m\}$.

Now, one can analyse the compact operator

$$D^{-1}P_0 \colon \operatorname{Ran} D \to L^2(\Omega).$$

Considering the decomposition (85) one obtains that

$$D^{-1}P_m$$

is a rank one operator such that $Du_m \mapsto u_m$. The operator norm of this rank one operator is

$$\|D^{-1}P_m\|^2 = \frac{\langle u_m, u_m \rangle}{\langle Du_m, Du_m \rangle_{\operatorname{Ran} D}}.$$

By an explicit calculation one can determine its order as

$$\|D^{-1}P_m\| = O(1/m),$$

and hence

$$\|D^{-1}P_m(D^*)^{-1}\| = O(1/m^2).$$

From a separation of variables analogous to the one presented in Subsection 5.3.1 one can derive that the singular values of $D^{-1}QM_{A^{-1}}Q^*(D^*)^{-1}$ can be numbered by two indices such that

$$s_{n,m}\left(D^{-1}QM_{A^{-1}}Q^*(D^*)^{-1}\right) = O(1/(n^2+m^2)), \quad n,m \in \mathbb{N},$$

just as in the case of the Dirichlet Laplacian on a rectangle. Hence the leading term of the counting functions of

$$D^{-1}(QM_AQ^*)^{-1}(D^*)^{-1} = D^{-1}QM_{A^{-1}}Q^*(D^*)^{-1} + c_0\, D^{-1}P_0(D^*)^{-1}$$

is determined only by the first addend which is discussed in Proposition 6.13 below. In particular it follows that the conjecture on the leading term of the eigenvalue counting functions is true in this particular case.

6.3. Comparison arguments

In the following the proofs of the above statements are carried out in several steps. The idea of the proofs is inspired by the line of approach which has been used by M. Š. Birman and M. Z. Solomyak in the article [17]. Instead of studying the operator $\mathcal{L}$, the inverse $\mathcal{L}^{-1}$ is considered, which is a compact self–adjoint operator and therefore accessible for variational methods. For compact operators variational methods are well studied, see for example [40].

The original eigenvalue problem $\lambda^{-1}\mathcal{L}u = u$ can be reformulated as a generalized eigenvalue problem involving the Dirichlet Laplacian $-\Delta_D = D^*D$ in $L^2(\Omega)$. Since $-\Delta_D$ as well as $\mathcal{L}$ are boundedly invertible there exists for each $u \in \mathrm{Dom}(\mathcal{L})$ exactly one $v \in \mathrm{Dom}(-\Delta_D)$ such that

$$\mathcal{L}u = -\Delta_D v \quad \text{and} \quad v = -\Delta_D^{-1}\mathcal{L}u. \tag{86}$$

Inserting this into (79) yields

LEMMA 6.10. *The eigenvalues $\pm\lambda_j^{\pm}$ of the operator $\mathcal{L}$ obey the following* min–max *principle*

$$\left(\lambda_{j+1}^{\pm}\right)^{-1} = \min_{\substack{\mathfrak{H}\subset\mathrm{Dom}(\Delta_D)\\ \mathrm{codim}\mathfrak{H}\le j}} \max_{\substack{v\in\mathfrak{H}\\ v\neq 0}} \pm\rho_0[v], \quad j \in \mathbb{N}_0,$$

where

$$\rho_0[v] = \frac{\langle Dv, (QM_AQ^*)^{-1}\, Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}}.$$

REMARK 6.11. *Since $-\Delta_D$ is a strictly positive and closed operator one can define the auxiliary Hilbert space $\mathcal{H}_{\Delta_D} = \mathrm{Dom}(\Delta_D)$, equipped with the scalar product $\langle\cdot,\cdot\rangle_{\Delta_D} = \langle\Delta_D\cdot,\Delta_D\cdot\rangle_{L^2(\Omega)}$. The map*

$$J\colon \mathcal{H}_{\mathcal{L}} \to \mathcal{H}_{\Delta_D}, \quad u \mapsto v = \Delta_D^{-1}\mathcal{L}u,$$

is unitary with the inverse

$$J^*\colon \mathcal{H}_{\Delta_D} \to \mathcal{H}_{\mathcal{L}}, \quad v \mapsto u = \mathcal{L}^{-1}\Delta_D v.$$

The substitution performed in (86) *is in fact an isometric isomorphism between Hilbert spaces. The form defined by ρ_0 defines a closed form in the Hilbert space $\mathcal{H}_{\Delta_D}$, which in turn determines an operator. This is unitarily equivalent to $\mathcal{L}_2^{-1}$ in $\mathcal{H}_{\mathcal{L}}$.*

PROOF OF THEOREM 6.3. Denote by T_+ the positive part and by T_- the negative part of a self–adjoint operator T. Hence

$$(QM_AQ^*)^{-1} = (QM_AQ^*)_+^{-1} + (QM_AQ^*)_-^{-1}$$

and there are positive (negative) eigenvalues of $\mathcal{L}$ if and only if QM_AQ^* has non–trivial positive (negative) part. For any $v \in \mathrm{Dom}(-\Delta_D)$ with $\rho_0[v] > 0$

$$\rho_0[v] = \frac{\langle Dv, (QM_AQ^*)^{-1}Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}} \leq \|(QM_AQ^*)_+^{-1}\| \frac{\langle Dv, Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}}$$

holds. Note that the quotient

$$\delta[v] = \frac{\langle Dv, Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}}, \quad v \in \mathrm{Dom}(\Delta_D)$$

defines a form which, in turn, determines an operator that is unitarily equivalent to $-\Delta_D^{-1}$. By [17, Lemma 1.2]

$$N^+(\lambda) \leq \|(QM_AQ^*)_+^{-1}\| N^+_{-\Delta_D}(\lambda),$$

where $N^+_{-\Delta_D}$ denotes the counting function for the Dirichlet Laplacian. The claim follows from the classical Weyl law, see [94]. For $N^-(\cdot)$ analogously. $\square$

PROOF OF THEOREM 6.8. Note that

$$H_0^2(\Omega_+) \oplus H_0^2(\Omega_-) \subset H_0^1(\Omega_+) \oplus H_0^1(\Omega_-) \subset H_0^1(\Omega).$$

Furthermore for any function $u \in H_0^2(\Omega_+) \oplus H_0^2(\Omega_-)$ one has $M_ADu = A(\cdot)\,\mathrm{grad}\,u$ and since $A_\pm(\cdot) \in C^\infty(\Omega_\pm)^{d\times d}$ and also $A_\pm(\cdot) \in L^\infty(\Omega;\mathbb{C})^{d\times d}$ one has $A(\cdot)\,\mathrm{grad}\,u \in E^2(\Omega)$, and hence
$-\mathrm{div}\,A(\cdot)\,\mathrm{grad}\,u \in L^2(\Omega)$. As $u \in H_0^1(\Omega)$ it follows by Theorem 5.4 (i) that $u \in \mathrm{Dom}(\mathcal{L})$. Now, consider the quotient

$$\rho[u] = \frac{\langle u, \mathcal{L}u\rangle}{\langle \mathcal{L}u, \mathcal{L}u\rangle} = \rho_+[u] + \rho_-[u], \quad \text{for } u \in H_0^2(\Omega_+) \oplus H_0^2(\Omega_-) \subset \mathrm{Dom}(\mathcal{L})$$

with

$$\rho_\pm[u] = \frac{\langle \mathrm{grad}\,u, A_\pm(\cdot)\,\mathrm{grad}\,u\rangle_{L^2(\Omega_\pm)^d}}{\langle \mathrm{div}\,A_\pm(\cdot)\,\mathrm{grad}\,u, \mathrm{div}\,A_\pm(\cdot)\,\mathrm{grad}\,u\rangle_{L^2(\Omega_\pm)}}.$$

The proof of the asymptotic inequality relies on a classical result by M. Š. Birman and M. Z. Solomyak [17, Theorems 3.2]. This result is formulated for a particular case, which is sufficient for the purpose of this exercise.

THEOREM 6.12. *Let $\mathcal{O} \subset \mathbb{R}^d$ be a bounded open set. Let $\mathfrak{a}$ and $\mathfrak{b}$ be sesquilinear forms satisfying the following assumptions*

(a) $\mathfrak{a}[u,u] = \sum_{|\alpha|=|\beta|=2} \int_{\mathcal{O}} a_{\alpha\beta}(x)\overline{D^\alpha u(x)} D^\beta u(x) dx,$
where $a_{\alpha\beta}(\cdot)$ are complex functions, such that the matrix $(a_{\alpha\beta}(x))_{\alpha\beta}$, $|\alpha| = |\beta| = 2$, is Hermitian and positive definite for almost every $x \in \mathcal{O}$, and the matrix valued functions $(a_{\alpha\beta}(\cdot))_{\alpha\beta}$ and $(a_{\alpha\beta}(\cdot))_{\alpha\beta}^{-1}$ are essentially bounded;

(b) $\mathfrak{b}[u,u] = \sum_{|\alpha|=|\beta|=1} \int_{\mathcal{O}} b_{\alpha\beta}(x)\overline{D^\alpha u(x)} D^\beta u(x)dx,$

where $b_{\alpha\beta}(\cdot)$ are essentially bounded functions satisfying $b_{\alpha\beta}(x) = \overline{b_{\beta\alpha}(x)}$ and $b_{\alpha\beta}(x)$ is sign–definite for almost all $x \in \mathcal{O}$.

Then the counting functions $N_{\mathcal{D}}^{\pm}(\lambda)$ of the Dirichlet critical values $\nu_{\mathcal{D},j}^{\pm}$ determined by the $\min - \max$ *principle,*

$$\left(\nu_{\mathcal{D},j}^{\pm}\right)^{-1} := \min_{\substack{\mathfrak{H}\subset H_0^2(\Omega)\\ \operatorname{codim}\mathfrak{H}\le j}} \max_{\substack{u\in\mathfrak{H}\\ u\neq 0}} \pm\frac{\mathfrak{b}[u,u]}{\mathfrak{a}[u,u]},$$

have the following asymptotics

$$N_{\mathcal{D}}^{\pm}(\lambda) \underset{\lambda\to\infty}{\sim} \lambda^{d/2}\frac{(2\pi)^{-d}}{d}\int_{\mathcal{O}}\int_{|\xi|=1}\left(\frac{(b(x,\xi))_\pm}{a(x,\xi)}\right)^{d/2} d\sigma(\xi)dx, \tag{87}$$

where $a(x,\xi)$ and $b(x,\xi)$ denote the symbols of the forms $\mathfrak{a}$ and $\mathfrak{b}$, respectively,

$$a(x,\xi) = \sum_{|\alpha|=|\beta|=2} a_{\alpha\beta}(x)\xi^{\alpha+\beta}, \quad b(x,\xi) = \sum_{|\alpha|=|\beta|=1} b_{\alpha\beta}(x)\xi^{\alpha+\beta}.$$

Consider the forms

$$\mathfrak{a}_\pm[u] = \langle \operatorname{div} A_\pm(\cdot)\operatorname{grad} u, \operatorname{div} A_\pm(\cdot)\operatorname{grad} u\rangle_{L^2(\Omega_\pm)}, \quad \text{for } u \in H_0^2(\Omega_\pm)$$

which have the symbols

$$a^\pm(x,\xi) = \left(\sum_{i,j=1}^d (A_\pm(x))_{i,j}\,\xi_i\xi_j\right)^2,$$

and

$$\mathfrak{b}_\pm[u] = \langle A_\pm(\cdot)\operatorname{grad} u, \operatorname{grad} u\rangle_{L^2(\Omega_\pm)}, \quad \text{for } u \in H_0^2(\Omega_\pm)$$

which have the symbols

$$b^\pm(x,\xi) = \sum_{i,j=1}^d (A_\pm(x))_{i,j}\,\xi_i\xi_j.$$

By assumption one has

$$\pm b^\pm(x,\xi) \ge \gamma(x)|\xi|^2, \quad \text{where } \gamma(x) = \|A^{-1}(x)\|^{-1},$$

compare for example [17, §2] and consequently also

$$a^\pm(x,\xi) \ge \gamma^2(x)|\xi|^4.$$

Hence the symbols $\pm b^\pm(x,\xi)$ and $a^\pm(x,\xi)$ are all strongly elliptic. Since $a^\pm(x,\xi)$ is a polynomial in ξ one can achieve the representation

$$a(x,\xi) = \sum_{|\alpha|=|\beta|=2} a_{\alpha\beta}(x)\xi^{\alpha+\beta}$$

for appropriate coefficients $a_{\alpha\beta}(x)$, where α and β are multi–indices. For $u \in C_0^\infty(\Omega_\pm)$ one obtains integrating by parts the representation

$$\mathfrak{a}_\pm[u] = \sum_{|\alpha|=|\beta|=2} \int_{\Omega_\pm} a^\pm_{\alpha\beta}(x)\overline{D^\alpha u(x)} D^\beta u(x) dx.$$

The concrete representation of $\mathfrak{a}_\pm[u]$ are not needed only the symbols. From the assumptions on $A_\pm(\cdot)$ it follows that the matrices $(a^\pm_{\alpha\beta}(x))_{\alpha\beta}$, $|\alpha| = |\beta| = 2$, are Hermitian and positive definite for almost every $x \in \Omega$, and furthermore the matrix valued functions $(a^\pm_{\alpha\beta}(\cdot))_{\alpha\beta}$ and $(a^\pm_{\alpha\beta}(\cdot))^{-1}_{\alpha\beta}$ are essentially bounded. Consequently the forms $\rho_\pm$ defined in $H^2_0(\Omega_\pm)$ satisfy all asummptions of Theorem 6.12. Hence

$$N^\pm_{\mathcal{D}}(\lambda)(\lambda) \sim \frac{(2\pi)^{-d}}{d}\omega^\pm \lambda^{d/2}, \quad \text{for } \lambda \to \infty,$$

where

$$\omega^\pm = \int_{\Omega_\pm} \int_{|\xi|=1} \left(\langle \xi, \pm A_\pm(x)\xi\rangle_{\mathbb{C}^d}\right)^{-d/2} d\sigma(\xi) dx,$$

with σ the Lebesgue measure on the unit sphere in $\mathbb{R}^d$. From the asymptotic distribution of the eigenvalues for elliptic operators, compare for example [1, Theorem 14.6], one reads that

$$N^\pm_{\mathcal{D}} \sim N_{\Omega_\pm} \quad \text{for } \lambda \to \infty.$$

The domain inclusion $H^2_0(\Omega_+) \oplus H^2_0(\Omega_-) \subset \operatorname{Dom}(\mathcal{L})$ implies together with the variational characterization of the eigenvalues in Proposition 6.1 that

$$\lambda^\pm_j \le \nu^\pm_{\mathcal{D},j} \quad \text{for } j \in \mathbb{N}$$

and consequently

$$N^\pm_{\mathcal{D}}(\lambda) \le N^\pm(\lambda) \quad \text{for } \lambda > 0.$$

□

Set

$$H_1 = QM_A^{-1}Q^* \quad \text{and} \quad H_2 = (QM_AQ^*)^{-1} - QM_A^{-1}Q^*.$$

One has $\rho_0[v] = \rho_1[v] + \rho_2[v]$ with

$$\rho_1[v] = \frac{\langle Dv, H_1 Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}} \quad \text{and} \quad \rho_2[v] = \frac{\langle Dv, H_2 Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}}.$$

Note that the operator $\mathcal{L}^{-1}$ admits the representation

$$\mathcal{L}^{-1} = D^{-1}(QM_AQ^*)^{-1}(D^*)^{-1}.$$

The decomposition

$$(QM_AQ^*)^{-1} = H_1 + H_2,$$

induces the decomposition

$$\mathcal{L}^{-1} = K_1 + K_2,$$

where

$$K_1 = D^{-1}H_1(D^*)^{-1} \quad \text{and} \quad K_2 = D^{-1}H_2(D^*)^{-1}.$$

Note that the form ρ_1 defines an operator that is unitarily equivalent to K_1 and analogously the form ρ_2 defines an operator that is unitarily equivalent to K_2. Hence, the eigenvalue problem for the operator K_1 can be reformulated as a generalized eigenvalue problem for differential operators of the type considered in [17]. How far the eigenvalues of $\mathcal{L}^{-1}$ differ from the eigenvalues of K_1 can be expressed in terms of K_2.

Denote by μ_j^+ and $-\mu_j^-$, $j \in \mathbb{N}$ the inverses of the positive and the inverses of the negative eigenvalues of K_1 enumerated in the increasing and decreasing order counting their multiplicities, respectively. With a slight abuse of notation let $N_{K_1}^{\pm}$ be the counting functions for the inverses of the positive and the inverses of the negative eigenvalues, which are defined by

$$N_{K_1}^{\pm}(\lambda) = \#\{\mu_j^{\pm} \leq \lambda\}.$$

Under additional assumptions on Ω one can determine the asymptotic behaviour of $N_{K_1}^{\pm}$.

PROPOSITION 6.13. *Suppose that Ω is either convex or has a C^2–boundary. Let $A(\cdot)$, $A(\cdot)^{-1} \in L^\infty(\Omega;\mathbb{C})^{d\times d}$ and let $A(x) = A^*(x)$ for almost all $x \in \Omega$. Then*

$$N_{K_1}^{\pm}(\lambda) \sim \frac{(2\pi)^{-d}}{d}\widetilde{\omega}^{\pm}\lambda^{d/2}, \quad \lambda \to \infty, \tag{88}$$

where

$$\widetilde{\omega}^{\pm} = \int_\Omega \int_{|\xi|=1} \left(\langle \xi, A(x)^{-1}\xi\rangle_{\mathbb{C}^d}\right)_{\pm}^{d/2} d\sigma(\xi)dx,$$

with $(t)_\pm := (|t| \pm t)/2$ and σ the Lebesgue measure on the unit sphere in $\mathbb{R}^d$.

The proof is postponed to the end of the section. For any compact operator K one can define the counting functions $N_K^{\pm}$ for the inverses of the non–zero eigenvalues analogous to the counting functions of K_1. Furthermore one can define the quantities

$$\delta_{\inf}^{\pm}(K) := \liminf_{\lambda\to\infty} N_K^{\pm}(\lambda)\,\lambda^{-d/2} \quad \text{and} \quad \delta_{\sup}^{\pm}(K) := \limsup_{\lambda\to\infty} N_K^{\pm}(\lambda)\,\lambda^{-d/2}. \tag{89}$$

If these quantities are finite and non-zero one writes

$$\delta_{\inf}^{\pm}(K)\lambda^{d/2} \lesssim N_K^{\pm}(\lambda) \lesssim \delta_{\sup}^{\pm}(K)\lambda^{d/2}, \quad \text{for } \lambda \to \infty,$$

and if $\delta_{\inf}^{\pm}(K) = \delta_{\sup}^{\pm}(K) =: \delta^{\pm}$ one writes

$$N_K^{\pm}(\lambda) \sim \delta^{\pm}\lambda^{d/2}, \quad \text{for } \lambda \to \infty.$$

LEMMA 6.14. *Assume that the conditions of Theorem 5.4 and the above Proposition 6.13 are fulfilled. Then there exist non–negative numbers $\delta_{\inf}^{\pm} \geq 0$ and $\delta_{\sup}^{\pm} \geq 0$ such that for any $\tau \in (0,1)$*

$$\tau^{d/2}N_{K_1}^{\pm}(\lambda) - \frac{\tau^{d/2}}{(1-\tau)^{-d/2}}\delta_{\inf}^{\mp}\lambda^{d/2} \lesssim N^{\pm}(\lambda) \lesssim \tau^{-d/2}N_{K_1}^{\pm}(\lambda) + (1-\tau)^{-d/2}\delta_{\sup}^{\pm}\lambda^{d/2},$$

holds asymptotically for $\lambda \to \infty$. Furthermore one has

$$\delta_{\inf}^{\pm} \leq \delta_{\inf}^{\pm}(K_2) \quad \textit{and} \quad \delta_{\sup}^{\pm} \leq \delta_{\sup}^{\pm}(K_2).$$

Note that assuming $\delta_{\inf}^{\pm} = 0$ and $\delta_{\sup}^{\pm} = 0$ one can take the limit $\tau \to 1$ and consequently $N_{K_1}^{\pm} \sim N^{\pm}$ for $\lambda \to \infty$. The function of Lemma 6.14 is to propose a measurement to quantify how far the counting functions $N^{\pm}$ can actually be from the counting functions $N_{K_1}^{\pm}$. For $A(\cdot) = \mathbb{1}_{\mathbb{C}^d}$ one has indeed $K_2 \equiv 0$ and Lemma 6.14 reproduces the classical Weyl law.

REMARK 6.15. *If H_2 is itself compact then $\delta^{\pm}_{\inf}(K_2) = \delta^{\pm}_{\sup}(K_2) = 0$ holds and consequently $N^{\pm}_{K_1} \sim N^{\pm}$ for $\lambda \to \infty$.*

PROOF OF LEMMA 6.14. Proposition 6.14 requires that both Theorem 5.4 and Proposition 6.13 can be applied. Theorem 6.3 implies that the limits

$$\delta^{\pm}_{\inf}(\mathcal{L}^{-1}) = \liminf_{j\to\infty} N^{\pm}(\lambda)\lambda^{-d/2} \quad \text{and} \quad \delta^{\pm}_{\sup}(\mathcal{L}^{-1}) = \limsup_{j\to\infty} N^{\pm}(\lambda)\lambda^{-d/2}$$

exist. For estimating the leading terms of the counting functions $N^{\pm}$ it is sufficient to find estimates on these quantities. Note that by Proposition 6.13

$$\delta^{\pm}_{\inf}(K_1) = \delta^{\pm}_{\sup}(K_1) = \frac{(2\,\pi)^{-d}}{d}\widetilde{\omega}^{\pm}.$$

Since

$$\mathcal{L}^{-1} = K_1 + K_2$$

one has for the counting functions

$$N^{\pm}(\lambda) \leq N^{\pm}_{K_1}(\tau\lambda) + N^{\pm}_{K_2}((1-\tau)\lambda), \quad \text{for } 0 < \tau < 1,$$

compare [17, Proof of Lemma 1.5 and the references given there]. Multiplying with $\lambda^{-d/2}$ and taking the limes superior gives

$$\delta^{\pm}_{\sup}(\mathcal{L}^{-1}) \leq \delta^{\pm}_{\sup}(K_1)\tau^{-d/2} + \delta^{\pm}_{\sup}(K_2)(1-\tau)^{-d/2}.$$

Using analogously

$$K_1 = \mathcal{L}^{-1} - K_2$$

by the same reasoning gives

$$N^{\pm}_{K_1}(\lambda) \leq N^{\pm}(\tau\lambda) + N^{\mp}_{K_2}((1-\tau)\lambda), \quad \text{for } 0 < \tau < 1.$$

Multiplying with $\lambda^{-d/2}$ and taking the limes inferior gives

$$\delta^{\pm}_{\inf}(K_1) \leq \delta^{\pm}_{\inf}(\mathcal{L}^{-1})\tau^{-d/2} + \delta^{\mp}_{\inf}(K_2)(1-\tau)^{-d/2}$$

and hence

$$\tau^{d/2}\delta^{\pm}_{\inf}(K_1) - \tau^{d/2}(1-\tau)^{-d/2}\delta^{\mp}_{\inf}(K_2) \leq \delta^{\pm}_{\inf}(\mathcal{L}^{-1}),$$

which proves the claim. □

PROOF OF THEOREM 6.6. By Proposition 5.5 the operator QM_AQ^* is boundedly invertible and hence the assumptions of Theorem 5.4 are fulfilled. Consequently there exists a unique self–adjoint operator $\mathcal{L}$ associated with $\mathfrak{l}$ and furthermore $\mathcal{L}$ is boundedly invertible with compact inverse.

Consider the form ρ_2, which is associated with an operator that is unitarily equivalent to K_2. Denote

$$P\colon L^2(\Omega) \to \operatorname{Ran} D, \quad Pu := \begin{cases} u, & u \perp \operatorname{Ran} D, \\ 0, & u \in \operatorname{Ran} D \end{cases}$$

and note that the adjoint operator $P^*\colon (\operatorname{Ran} D)^{\perp} \to L^2(\Omega)$ is the embedding of $(\operatorname{Ran} D)^{\perp}$ in $L^2(\Omega)$. Recall that for dimension $d = 1$ the space $(\operatorname{Ran} D)^{\perp}$ is the space of constant functions in $L^2(\Omega)$. The decomposition $L^2(\Omega) = \operatorname{Ran} D \oplus (\operatorname{Ran} D)^\perp$ induces a block structure on M_A as well as on M_A^{-1} and hence one has

$$\begin{bmatrix} QM_AQ^* & QM_AP^* \\ PM_AQ^* & PM_AP^* \end{bmatrix} \begin{bmatrix} QM_A^{-1}Q^* & QM_A^{-1}P^* \\ PM_A^{-1}Q^* & PM_A^{-1}P^* \end{bmatrix} = \begin{bmatrix} \mathbb{1}_{\operatorname{Ran} Q} & 0 \\ 0 & \mathbb{1}_{\operatorname{Ran} P} \end{bmatrix}.$$

From this one obtains

$$QM_AQ^*QM_A^{-1}Q^* + QM_AP^*PM_A^{-1}Q^* = \mathbb{1}_{\operatorname{Ran} Q}$$

and consequently

$$(QM_AQ^*)^{-1} - QM_A^{-1}Q^* = (QM_AQ^*)^{-1}QM_AP^*PM_A^{-1}Q^*,$$

which gives

$$\begin{aligned} \rho_2[v] &= \frac{\left\langle \left[(QM_AQ^*)^{-1} - QM_A^{-1}Q^*\right] Dv, Dv \right\rangle_{L^2(\Omega)}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}} \\ &= \frac{\left\langle PM_A^{-1}Q^*Dv, PM_AQ^* \left(QM_AQ^*\right)^{-1} Dv \right\rangle_{L^2(\Omega)}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}}. \end{aligned}$$

Thus, in dimension $d = 1$ the operator K_2 is a rank one operator, since P has rank one, and therefore

$$\delta^{\pm}_{\inf}(K_2) = \delta^{\pm}_{\sup}(K_2) = 0.$$

Applying Lemma 6.14 and taking the limit $\tau \to 1$ proves that

$$N^{\pm}_{K_1} \sim N^{\pm}, \quad \text{for } \lambda \to \infty.$$

Observing that in dimension $d = 1$ one has always $\widetilde{\omega}^{\pm} = \omega^{\pm}$ finishes the proof. □

It remains to determine the asymptotic behaviour of the eigenvalue counting functions of K_1. As already remarked the operator K_1 can be associated with the form ρ_1 which is defined by

$$\rho_1[v] = \frac{\langle Dv, M_A^{-1}Dv\rangle_{L^2(\Omega)^d}}{\langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}} \quad \text{with } v \in \operatorname{Dom}(-\Delta_D).$$

LEMMA 6.16. *The non-zero eigenvalues* $(\pm\mu_j^{\pm})^{-1}$ *of the operator* K_1 *obey the following* min–max *principle*

$$\left(\mu^{\pm}_{j+1}\right)^{-1} = \min_{\substack{\mathfrak{H}\subset \operatorname{Dom}(\Delta_D) \\ \operatorname{codim}\mathfrak{H}\le j}} \max_{\substack{v\in\mathfrak{H} \\ v\neq 0}} \pm\rho_1[v], \quad j \in \mathbb{N}_0.$$

PROOF. The operator

$$K_1 = D^{-1}QM_A^{-1}Q^*(D^*)^{-1}$$

is compact and therefore its non–zero eigenvalues can be determined as the successive extrema of the ratio

$$\rho_{K_1}[w] = \frac{\langle w, K_1 w\rangle_{L^2(\Omega)}}{\langle w, w\rangle_{L^2(\Omega)}}, \quad w \in L^2(\Omega),\ w \neq 0.$$

Substituting $w = -\Delta_D v$ with $v \in \operatorname{Dom}(-\Delta_D)$ gives

$$\rho_{K_1}[w] = \rho_1[v].$$

The form ρ_1 defines in the Hilbert space $\mathcal{H}_{\Delta_D}$ an operator that is unitarily equivalent to K_1. To determine the non–zero eigenvalues one applies the $\min$–$\max$–principle to ρ_1. $\square$

Under the assumptions of Proposition 6.13 one has

$$\mathrm{Dom}(\Delta_D) = H_0^1(\Omega) \cap H^2(\Omega), \tag{90}$$

see for example [42, Theorems 2.2.2.3 and 3.2.1.2] or [73, Chapter II.§7 Remark 7.1] and the second fundamental inequality for elliptic operators

$$\|u\|_{H^2(\Omega)} \leq C_\Omega \Delta_D u, \quad u \in \mathrm{Dom}(\Delta_D), \quad C_\Omega > 0, \tag{91}$$

see [73, Chapter II.§6 equation (6.29) and Remark 6.1] holds.

Let $\alpha, \beta \in \mathbb{N}_0^d$ be multi indices and $|\alpha| = \alpha_1 + \cdots + \alpha_d$. For any $\epsilon \geq 0$ one sets

$$\begin{aligned} \mathfrak{a}_\epsilon[v,v] &= \langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)} + \epsilon \sum_{|\alpha|=|\beta|=2} \frac{2\epsilon}{\alpha!}\delta_{\alpha\beta} \int_\Omega \overline{D^\alpha v(x)} D^\beta v(x) dx \\ &= \sum_{|\alpha|=|\beta|=2} a_{\alpha\beta}(\epsilon) \int_\Omega \overline{D^\alpha v(x)} D^\beta v(x) dx, \quad v \in H_0^1(\Omega) \cap H^2(\Omega), \end{aligned} \tag{92}$$

with

$$a_{\alpha\beta}(\epsilon) := a_{\alpha\beta}(0) + \frac{2\epsilon}{\alpha!}\delta_{\alpha\beta},$$

and

$$a_{\alpha\beta}(0) := \begin{cases} 1, & |\alpha|_\infty = 2 \quad \text{or} \quad |\beta|_\infty = 2, \\ 0, & \text{else,} \end{cases}$$

where $|\alpha|_\infty := \max_{i=1,\dots,d} \alpha_i$. The matrix $(a_{\alpha\beta}(0))_{\alpha\beta}$ corresponds to the quadratic form

$$\mathfrak{a}_0[v,v] = \sum_{|\alpha|=|\beta|=2} a_{\alpha\beta}(0) \int_\Omega \overline{D^\alpha v(x)} D^\beta v(x) dx = \langle \Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}.$$

For a differential quadratic form $\mathfrak{a}$ defined by

$$\mathfrak{a}[v,v] = \sum_{\alpha,\beta \in I} a_{\alpha\beta}(x) \int_\Omega \overline{D^\alpha v(x)} D^\beta v(x) dx$$

on $\Omega \subset \mathbb{R}^d$, where I is a set of multi–indices, the *symbol* $a(x,\cdot)$ *of* $\mathfrak{a}$ is defined, independently of its domain, as the function $a(\cdot,\cdot)$ given by

$$a(x,\xi) = \sum_{\alpha,\beta \in I} a_{\alpha\beta}(x)\xi^\alpha \xi^\beta, \quad \xi \in \mathbb{R}^d, \quad x \in \Omega.$$

Observe that for $\epsilon > 0$ the matrix with entries $(a_{\alpha\beta}(\epsilon))_{\alpha\beta}$, where $|\alpha|, |\beta| = 2$, is positive definite and the symbol of the quadratic form $\mathfrak{a}_\epsilon$ given by (92) is

$$a_\epsilon(\xi) = \sum_{|\alpha|,|\beta|=2} a_{\alpha\beta}(\epsilon)\xi^{\alpha+\beta} = (1+\epsilon)|\xi|^4, \quad \xi \in \mathbb{R}^d.$$

The change from $\mathfrak{a}_0[\cdot,\cdot]$ to $\mathfrak{a}_\epsilon[\cdot,\cdot]$, for $\epsilon > 0$, equates to a perturbation of the metric given by $\mathfrak{a}_0[\cdot,\cdot]$ in $\mathrm{Dom}(\Delta_D)$. This means that there is a perturbation of the metric in the Hilbert space $\mathcal{H}_{\Delta_D}$. Eventually it turns out that this perturbation has only small effects on the leading terms of the eigenvalue asymptotics of the operator considered, since the leading terms depend only on the symbol of the form.

LEMMA 6.17. *For $\epsilon > 0$ let*

$$\left(\nu_{j+1}^{\pm}(\epsilon)\right)^{-1} := \min_{\substack{\mathfrak{H}\subset H_0^1(\Omega)\cap H^2(\Omega)\\ \operatorname{codim}\mathfrak{H}\le j}} \max_{\substack{v\in\mathfrak{H}\\ v\neq 0}} \pm\frac{\langle Dv, M_A^{-1}Dv\rangle_{L^2(\Omega)^d}}{\mathfrak{a}_\epsilon[v,v]}, \quad j\in\mathbb{N}_0.$$

Then the counting functions

$$N_\epsilon^{\pm}(\lambda) := \#\{\nu_j^{\pm}(\epsilon) < \lambda\}$$

have the asymptotics

$$N_\epsilon^{\pm}(\lambda) \underset{\lambda\to\infty}{\sim} \lambda^{d/2}\frac{(2\pi)^{-d}}{d}(1+\epsilon)^{-d/2}\int_\Omega\int_{|\xi|=1}\left(\langle\xi, A(x)^{-1}\xi\rangle_{\mathbb{C}^d}\right)_{\pm}^{d/2} d\sigma(\xi)dx \tag{93}$$

with $(t)_\pm := (|t|\pm t)/2$ and σ the Lebesgue measure on the unit sphere in $\mathbb{R}^d$.

The proof of the lemma relies on classical results by M. Š. Birman and M. Z. Solomyak [17, Theorems 3.4 and 3.5]. These results are formulated for a particular case, which is sufficient for the purpose of this chapter.

THEOREM 6.18. *Let $\mathcal{O}\subset\mathbb{R}^n$ be a bounded open set. Let $\mathfrak{a}[u,u]$ and $\mathfrak{b}[u,u]$ be sesquilinear forms satisfying the following assumptions*

(a) $\mathfrak{a}[u,u] = \sum_{|\alpha|=|\beta|=2}\int_{\mathcal{O}} a_{\alpha\beta}\overline{D^\alpha u(x)}D^\beta u(x)dx$, *where $a_{\alpha\beta}$ are complex numbers satisfying $a_{\alpha\beta}=\overline{a_{\beta\alpha}}$;*
(b) *the matrix $(a_{\alpha\beta})_{\alpha\beta}$, $|\alpha|=|\beta|=2$, is positive definite;*
(c) $\mathfrak{b}[u,u] = \sum_{|\alpha|=|\beta|=1}\int_{\mathcal{O}} b_{\alpha\beta}(x)\overline{D^\alpha u(x)}D^\beta u(x)dx$, *where $b_{\alpha\beta}(x)$ are essentially bounded functions satisfying $b_{\alpha\beta}(x)=\overline{b_{\beta\alpha}(x)}$ for almost all $x\in\mathcal{O}$.*

Then the counting functions $N_{\mathcal{D}}^{\pm}(\lambda,t)$ of the Dirichlet critical values $\nu_{\mathcal{D},j}^{\pm}$ determined by the min–max *principle,*

$$\left(\nu_{\mathcal{D},j}^{\pm}(t)\right)^{-1} := \min_{\substack{\mathfrak{H}\subset H_0^2(\mathcal{O})\\ \operatorname{codim}\mathfrak{H}\le j}} \max_{\substack{u\in\mathfrak{H}\\ u\neq 0}} \pm\frac{\mathfrak{b}[u,u]}{\mathfrak{a}[u,u]+t\|u\|^2}, \quad t\ge 0,$$

have the following asymptotics

$$N_{\mathcal{D}}^{\pm}(\lambda,t) \underset{\lambda\to\infty}{\sim} \lambda^{d/2}\frac{(2\pi)^{-d}}{d}\int_{\mathcal{O}}\int_{|\xi|=1}\left(\frac{(b(x,\xi))_\pm}{a(\xi)}\right)^{d/2} d\sigma(\xi)dx, \tag{94}$$

where $a(\xi)$ and $b(x,\xi)$ denote the symbols of the forms $\mathfrak{a}$ and $\mathfrak{b}$, respectively,

$$a(\xi) = \sum_{|\alpha|=|\beta|=2} a_{\alpha\beta}\xi^{\alpha+\beta}, \quad b(x,\xi) = \sum_{|\alpha|=|\beta|=1} b_{\alpha\beta}(x)\xi^{\alpha+\beta}.$$

If, in addition, $\mathcal{O}$ has a Lipschitz boundary, then the counting functions $N^{\pm}_{\mathcal{N}}(\lambda,t)$ of the Neumann critical values $\nu^{(\pm)}_{\mathcal{N},j}(t)$ determined by

$$\left(\nu^{\pm}_{N,j}(t)\right)^{-1} := \min_{\substack{\mathcal{L}\subset H^2(\mathcal{O})\\ \operatorname{codim}\mathcal{L}\leq j}} \max_{\substack{u\in\mathcal{L}\\ u\neq 0}} \pm\frac{\mathfrak{b}[u,u]}{\mathfrak{a}[u,u]+t\|u\|^2}, \quad t>0,$$

have the asymptotics (94).

Note that Theorem 6.18 cannot be applied directly to the quotient ρ_0. This is due to the fact that the form defined by $\langle\Delta_D v, \Delta_D v\rangle$, $v\in\operatorname{Dom}(-\Delta_D)\subset L^2(\Omega)$ is associated with the operator Δ_D^2, which is not exactly the classical bi–Laplace operator. This is illustrated for dimension $d=2$, where one has

$$\langle\Delta_D v, \Delta_D v\rangle_{L^2(\Omega)} = \left\langle D^2 v, a(0)D^2 v\right\rangle_{L^2(\Omega)^3}, \quad \text{where} \quad a(0) = \begin{bmatrix} 1 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 1\end{bmatrix}$$

and the bi–gradient D^2 is given by

$$D^2 v = \begin{bmatrix} D^{(2,0)}v\\ D^{(1,1)}v\\ D^{(0,2)}v\end{bmatrix} \quad \text{with} \quad D^{(i,j)}v = \frac{d^2 w}{dx_i dx_j}, \quad i,j\in\{0,1,2\}.$$

The matrix $a(0)$ has the eigenvalues 2 and 0, and is clearly not elliptic. One is tempted to interchange the orders of the derivatives, but this is prohibited by the boundary values of $v\in\operatorname{Dom}(-\Delta_D) = H^2(\Omega)\cap H^1_0(\Omega)$. In contrast, bi–Laplace operators are defined by elliptic forms which are given by expressions

$$\left\langle D^2 v, a' D^2 v\right\rangle_{L^2(\Omega)^3} \quad \text{with} \quad a' = \begin{bmatrix} 1 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 1\end{bmatrix}.$$

A form that is accessible by Theorem 6.18 and which is close to the form defined by $\langle\Delta_D v, \Delta_D v\rangle_{L^2(\Omega)}$ is the form $\mathfrak{a}_\epsilon$ defined using the matrix $a(0)+\epsilon a'$, for $\epsilon>0$. As already remarked this corresponds to a small perturbation of the metric in the Hilbert space $\mathcal{H}_{\Delta_D}$.

PROOF OF LEMMA 6.17. Denote by

$$\left(\nu^{\pm}_{\mathcal{D},j,t}(\epsilon)\right)^{-1}, \quad \left(\nu^{\pm}_{j,t}(\epsilon)\right)^{-1} \quad \text{and} \quad \left(\nu^{\pm}_{\mathcal{N},j,t}(\epsilon)\right)^{-1}$$

the quantities determined by the $\min-\max$ principle

$$\min_{\substack{\mathfrak{H}\subset\mathcal{S}\\ \operatorname{codim}\mathfrak{H}\leq j}} \max_{\substack{u\in\mathfrak{H}\\ u\neq 0}} \pm\frac{\mathfrak{b}[u,u]}{\mathfrak{a}_\epsilon[u,u]+t\|u\|^2}, \quad t>0,$$

with $\mathcal{S}$ chosen to be

$$H^2_0(\Omega), \quad H^1_0(\Omega)\cap H^2(\Omega) \quad \text{and} \quad H^2(\Omega),$$

respectively. Here the form $\mathfrak{a}_\epsilon$ is defined in (92). Obviously, for all $t>0$ and $\epsilon>0$ these numbers satisfy the inequality

$$\nu^{\pm}_{\mathcal{D},j,t}(\epsilon) \geq \nu^{\pm}_{j,t}(\epsilon) \geq \nu^{\pm}_{\mathcal{N},j,t}(\epsilon).$$

Applying Theorem 6.18 yields that for all $t > 0$ the counting functions

$$N_{\epsilon,t}(\lambda) := \#\{\nu^{\pm}_{j,t}(\epsilon) \le \lambda\}$$

obey the asymptotics (93). Since the asymptotics are independent of t, the claim follows. □

PROOF OF PROPOSITION 6.13. Pick an arbitrary $\epsilon > 0$. Observe that

$$\mathfrak{a}_\epsilon[v,v] \ge \mathfrak{a}_0[v,v]$$

for all $v \in H^1_0(\Omega) \cap H^2(\Omega)$, which implies the inequality

$$\nu^{\pm}_j(\epsilon) \ge \lambda^{\pm}_j. \tag{95}$$

Under the assumptions of Proposition 6.13 the second fundamental inequality for elliptic operators

$$\|v\|_{H^2(\Omega)} \le C_\Omega \|\Delta v\|_{L^2(\Omega)}, \qquad v \in H^1_0(\Omega) \cap H^2(\Omega),$$

holds, see [73, Section II.6, in particular Remark 6.1]. This implies that there is a constant, denoted by the same symbol, $C_\Omega > 0$, such that

$$\sum_{|\alpha|=2} \frac{2}{\alpha!} \int_\Omega \overline{D^\alpha v(x)} D^\alpha v(x) dx \le C_\Omega \|\Delta v\|^2_{L^2(\Omega)}$$

holds for all $v \in H^1_0(\Omega) \cap H^2(\Omega)$. Thus, taking into account the definition of $\mathfrak{a}_\epsilon$ one has that

$$\mathfrak{a}_\epsilon[v,v] \le (1 + \epsilon C_\Omega)\mathfrak{a}_0[v,v]$$

holds for all $v \in H^1_0(\Omega) \cap H^2(\Omega)$. This implies

$$\nu^{\pm}_j(\epsilon) \le (1 + \epsilon C_\Omega)\mu^{\pm}_j. \tag{96}$$

Combining (95) with (96) one gets to the two-sided estimate

$$(1 + \epsilon C_\Omega)^{-1} \nu^{\pm}_j(\epsilon) \le \mu^{\pm}_j \le \nu^{\pm}_j(\epsilon), \quad \text{for any} \quad \epsilon > 0.$$

From the inequality for the eigenvalues one obtains the converse inequality for the corresponding counting functions $N^{\pm}_{K_1}$ and $N^{\pm}_\epsilon$, which therefore obey the inequality

$$N^{\pm}_\epsilon(\lambda) \le N^{\pm}_{K_1}(\lambda) \le N^{\pm}_\epsilon((1 + \epsilon C_\Omega)\lambda), \quad \epsilon > 0.$$

Now by Lemma 6.17 it follows that for any $\epsilon > 0$

$$\liminf_{\lambda\to\infty} \lambda^{-d/2} N^{\pm}_{K_1}(\lambda) \ge \frac{(2\pi)^{-d}}{d}(1+\epsilon)^{-d/2} \int_\Omega \int_{|\xi|=1} \left(\langle \xi, A(x)^{-1}\xi\rangle_{\mathbb{C}^d}\right)^{d/2}_{\pm} d\sigma(\xi) dx$$

and

$$\limsup_{\lambda\to\infty} \lambda^{-d/2} N^{\pm}_{K_1}(\lambda) \le \frac{(2\pi)^{-d}}{d} \frac{(1+\epsilon C_\Omega)^{d/2}}{(1+\epsilon)^{d/2}} \int_\Omega \int_{|\xi|=1} \left(\langle \xi, A(x)^{-1}\xi\rangle_{\mathbb{C}^d}\right)^{d/2}_{\pm} d\sigma(\xi) dx,$$

which implies the asymptotic formulae for $N^{\pm}_{K_1}$, that are given in equation (88). □

Conclusions and outline

The main outcome of this work concerns different fields and basically, the different topics of this thesis can be understood on their own. The main results are summarized in the following.

In the first part three different kinds of differential operators on metric graphs have been considered. The study of Laplace operators on metric graphs is well developed. However, not all questions related to this topic are completely answered. This work closes two gaps that still were open. A complete characterisation of the quasi–m–accretive Laplace operators on finite metric graphs has been derived in terms of boundary conditions. As a specification the m–accretive Laplace operators on finite metric graphs have been characterized as well. This gives rise to solutions of the diffusion equation on graphs in terms of quasi–contractive or even contractive semigroups.

The negative spectrum of self–adjoint Laplace operators on finite metric graphs has been analysed in detail and the knowledge about the negative eigenvalues has been refined. Three different types of estimates from below and from above on each of the negative eigenvalues have been derived. The cases where the resulting lower bounds on the spectrum are optimal have been characterised as well. As an application of this, one obtains two–sided estimates on the growth bound of quasi–contractive semigroups generated by quasi–m–accretive Laplace operators.

Instead of the Laplacian one can consider an operator which is given on some edges by the first and on some other edges by the second derivative operator. The coupling takes place only at the vertices and is implemented in terms of boundary conditions. For compact metric graphs a class of boundary conditions is exhibited which yield quasi–m–dissipative operators. The spectral theory of these operators gives information on the semigroups generated by them. These semigroups describe a time evolution which is on some edges given by the transport equation and on some edges by the diffusion equation. The simultaneous consideration of dynamics of different types is a new aspect in the theory of differential operators of metric graphs.

Indefinite differential operators arise in different contexts. As a new model problem, an indefinite second order differential operator is introduced which is "plus Laplace" on some edges and "minus Laplace" on some other edges. The boundary conditions which define self–adjoint realisations are completely characterized. The spectral and scattering theory for these self–adjoint realisations is elaborated in detail. The spectrum resembles the spectrum of the sum of a positive Laplacian and a Laplacian multiplied by minus one. The scattering properties of this indefinite system show specific and unusual features.

The second part of this work deals with self–adjoint indefinite second order differential operators on bounded domains associated with indefinite quadratic forms. The main result is that in dimension $d = 1$ asymptotically these operators resemble the spectrum of the sum of a positive definite and a negative definite operator. This is reflected by the asymptotic behaviour of the eigenvalues which satisfy, for $d = 1$ a generalized Weyl law. For dimension $d \geq 2$ the order of the counting functions is $\lambda^{d/2}$ and in specific situations the conjectured generalized Weyl law is at least a lower bound on the counting functions. The proofs are based on the application of variational methods to unbounded and indefinite self–adjoint operators.

So, what are the conclusions of this thesis? In short two things. First, differential operators on metric graphs can serve as simplified and exactly solvable models in various situations, and over and above starting with metric graphs can ease the first steps to introduce new mathematical models. The second conclusion is that indefinite second order differential operators on bounded domains decompose into two "classes". The class of well behaved operators keeps many properties from their sign definite and elliptic relatives like the compactness of the resolvent, the asymptotic behaviour of the eigenvalues and some of their relations to forms. The behaviour of the operators that do not lie in this category cannot be predicted in general.

Unfortunately there is no criterion available for dimensions larger than one to decide when an indefinite operator fits into the scheme presented here. More generally, one can ask about those indefinite operators which resemble the sum of a positive operator and a negative operator, and about those which do not exhibit such a feature. Part 2 has dealt almost only with the well behaved indefinite second order differential operators and only in Section 5.3 of Chapter 5 the "outsiders" have been mentioned.

In retrospect one could not expect even that there are actually such well behaved indefinite differential operators and new problems and questions arise naturally. Does the asymptotic behaviour of the eigenvalues always satisfy the conjectured generalized Weyl law? If yes, can one give sense to lower order terms in the eigenvalue asymptotics and what should one expect from them? Can the assumptions of the representation theorem be weakened? It has been exhibited that regularised problems can always be considered. So, the convergence properties are of interest in particular for the case when it is not clear what the limit operator actually is.

The study of simplified models on graphs left many questions open for the models themselves, but also for their perspective. After many spectral properties of Laplace operators on finite metric graphs have been derived in the last decades, the direction goes perspicuously to locally finite or more general infinite graphs. However, there is still room for optimization of the results already obtained for finite graphs, also with the perspective to take limits of finite graphs. An exemplary problem is the one of the lower bound on the spectrum. In the theory of point interactions the problem whether a Laplacian with δ or δ' interactions on a line or a half–line is semi–bounded becomes a complicated and non–transparent task whenever the edges' lengths are shrinking to zero. Here a better study of the lower bounds on finite graphs with positive, but small edge lengths can shed light on the mechanisms of this problem.

For the mixed transport and diffusion system it is clearly very interesting to point out natural matching conditions at the vertices. In general I believe that the study of coupled dynamics of different types has the best chances to become practically relevant and to enrich the tool box of natural scientists with new and more flexible features. The question how to carry this over to higher dimensions is as natural as to ask for non–linear versions.

The model problem of an indefinite second order operator on a metric graph has played a specific role as it is closely related to the problem discussed in Part 2. Besides many technical questions that are left open, particularly the scattering theory for the problem has left much space for further research. The scattering data make it possible to compare the characteristics of this new model problem to the well studied subject of Laplacians on metric graphs. This could become interesting for the understanding of cloaking phenomena in some contexts, as an observer of a physical system is tempted to suppose the usual model, here for example the Helmholtz equation involving the usual Laplacian, but the device is in fact governed by another dynamics that might feign features of the usual one. In this context the behaviour of the scattering matrix for small as well as for large frequencies is of great interest. However it is even not clear that these limits always exist. As usually...

...Vorhang zu und alle Fragen offen.[1]

[1]"[...]curtain closed and all questions open.", is a citation from *Bertolt Brecht: Der Gute Mensch von Sezuan.*

APPENDIX A

PROOF OF PROPOSITION 4.26. In order to prove that the kernel $r(\cdot,\cdot,k)$ defines the resolvent operator $(T(A,B)-k^2)^{-1}$ one has to check:

(i) $(T^{\max}-k^2)\int_{\mathcal{G}} r(x,y,k)\varphi(y)=\varphi(x)$ for all $\varphi\in\mathcal{H}$,

(ii) $R(k^2)\varphi=\int_{\mathcal{G}} r(x,y,k)\varphi(y)\in\operatorname{Dom}(T(A,B))$ for $\varphi\in\mathcal{H}$ and

(iii) $r(x,y,-\overline{k})=r(y,x,k)^*$ holds for $\operatorname{Im}k>0$.

The statements (i) and (ii) prove that $R(k^2)$ is the left inverse of $T(A,B)-k^2$. To prove that it is also the right inverse it is sufficient to verify (iii). The proofs of (i) and (ii) are given for $k\in\mathcal{Q}$ with (iii) the claim carries over to $k\in\mathcal{P}$.

Proof of (i): For $\varphi\in\mathcal{H}$ with $\varphi_j\in C_0^\infty(I_j,\mathbb{C})$ for every $j\in\mathcal{E}\cup\mathcal{I}$, one uses that the Green's function to the problem is known and one has

$$\begin{aligned}
\left(-\frac{d^2}{dx^2}-k^2\right)\int_{I_j}\frac{i}{2k}e^{ik|x_j-y_j|}\varphi_j(y_j)dy_j &=\varphi_j(x_j), && \text{for } k\in\mathcal{Q}\cup\mathcal{P},\\
-\left(+\frac{d^2}{dx^2}-k^2\right)\int_{I_j}\frac{1}{2k}e^{-k|x_j-y_j|}\varphi_j(y_j)dy_j &=\varphi_j(x_j), && \text{for } k\in\mathcal{Q} \text{ and}\\
-\left(+\frac{d^2}{dx^2}-k^2\right)\int_{I_j}\frac{1}{2k}e^{k|x_j-y_j|}\varphi_j(y_j)dy_j &=\varphi_j(x_j), && \text{for } k\in\mathcal{P}.
\end{aligned}$$

Since the kernel $r^0_{n,m}(x,y,k,i\kappa)$ defines a bounded operator in $\mathcal{H}$, by continuous continuation from

$$\mathcal{D}'=\bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} C_0^\infty(I_j,\mathbb{C})$$

to $\mathcal{H}$ it follows that for $k\in\mathcal{Q}$ and for all $\varphi\in\mathcal{H}$

$$\left(T^{\max}-k^2\right)\int_{\mathcal{G}} r^0(x,y,k,ik)\varphi(y)dy=\varphi(x)$$

holds. Observe furthermore that

$$\left(T^{\max}-k^2\right)\int_{\mathcal{G}} r^1(x,y,k,ik)\varphi(y)dy=0$$

which completes the proof.

Proof of (ii): Observe that

$$\int_{\mathcal{G}} r^0(x,y,k,i\kappa)\varphi(y)\in\mathcal{D}\quad\text{and}\quad\int_{\mathcal{G}} r^1(x,y,k,i\kappa)\varphi(y)\in\mathcal{D},$$

and hence

$$R(k^2)\varphi = \int_{\mathcal{G}} r(\cdot, y, k)\varphi(y) \in \mathcal{D} = \mathrm{Dom}(T^{\max}).$$

Let be $k \in \mathcal{Q}$ and consider the traces for the free Green's function $r^0(\cdot,\cdot,k,i\kappa)$. One has

$$\begin{aligned}
\underline{\int_{\mathcal{G}} r_0(x,y,k,i\kappa)f(y)} =& R^+_{n,m}(k,i\kappa,\underline{a})^{-1} J_{n,m}\hat{f}(k,i\kappa),\\
\underline{\left(\int_{\mathcal{G}} r_0(x,y,k,i\kappa)f(y)\right)'} =& I_{n,m}(k,i\kappa)R^+_{n,m}(k,i\kappa,\underline{a})^{-1} J_{n,m}\hat{f}(k,i\kappa)
\end{aligned}$$

with

$$\hat{f}(k,i\kappa) := \int_{\mathcal{G}} \Phi_{n,m}(y,k,i\kappa)W_{n,m}(k,i\kappa)f(y)dy.$$

Since the free Green's function decouples the positive from the negative edges the above statement follows already from the corresponding calculation for self–adjoint Lapalce operators, compare [63, Proof of Lemma 4.2]

For the correction term $r^1(\cdot,\cdot,k,i\kappa)$ observe that for an appropriate vector f one has the traces

$$\underline{\begin{bmatrix} e^{ikx} & 0 & 0 \\ 0 & e^{ikx} & e^{-ikx} \end{bmatrix} \begin{bmatrix} f_{\mathcal{E}} \\ f_{\mathcal{I}_-} \\ f_{\mathcal{I}_+} \end{bmatrix}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & e^{ik\underline{a}} & e^{-ik\underline{a}} \end{bmatrix} \begin{bmatrix} f_{\mathcal{E}} \\ f_{\mathcal{I}_-} \\ f_{\mathcal{I}_+} \end{bmatrix},$$

$$\underline{\begin{bmatrix} e^{ikx} & 0 & 0 \\ 0 & e^{ikx} & e^{-ikx} \end{bmatrix} \begin{bmatrix} f_{\mathcal{E}} \\ f_{\mathcal{I}_-} \\ f_{\mathcal{I}_+} \end{bmatrix}'} = \begin{bmatrix} ik & 0 & 0 \\ 0 & ik & -ik \\ 0 & -ike^{ik\underline{a}} & ike^{-ik\underline{a}} \end{bmatrix} \begin{bmatrix} f_{\mathcal{E}} \\ f_{\mathcal{I}_-} \\ f_{\mathcal{I}_+} \end{bmatrix},$$

and therefore

$$\underline{\Phi_{n,m}(x,k,i\kappa)\hat{f}} = X_{n,m}(k,i\kappa)\hat{f}, \qquad \underline{\left(\Phi_{n,m}(x,k,i\kappa)\hat{f}\right)'} = Y_{n,m}(k,i\kappa)\hat{f},$$

where $\hat{f}$ is here short for $\hat{f}(k,i\kappa)$, compare also [63, Proof of Lemma 4.2]. This gives the traces of the correction term

$$\underline{\int_{\mathcal{G}} r_1(x,y,k,i\kappa)f(y)} = X_{n,m}(k,i\kappa)G_{n,m}(k,i\kappa,\underline{a})\hat{f}$$

and

$$\underline{\left(\int_{\mathcal{G}} r_1(x,y,k,i\kappa)f(y)\right)'} = Y_{n,m}(k,i\kappa)G_{n,m}(k,i\kappa,\underline{a})\hat{f}.$$

Together one has

$$\begin{aligned}&\underline{A\int_{\mathcal{G}} r^0(x,y,k,i\kappa)f(y)} + \underline{B\Big(\int_{\mathcal{G}} r^0(x,y,k,i\kappa)f(y)\Big)'}\\ +&\underline{A\int_{\mathcal{G}} r^1(x,y,k,i\kappa)f(y)} + \underline{B\Big(\int_{\mathcal{G}} r^1(x,y,k,i\kappa)f(y)\Big)'}\end{aligned}$$

$$\begin{aligned}=&AR^+_{n,m}(k,i\kappa,\underline{a})^{-1}J_{n,m}\hat{f} + BI_{n,m}(k,i\kappa)R^+_{n,m}(k,i\kappa,\underline{a})^{-1}J_{n,m}\hat{f}\\ &+AX_{n,m}(k,i\kappa)G_{n,m}(k,i\kappa,\underline{a})\hat{f} + BY_{n,m}(k,i\kappa)G_{n,m}(k,i\kappa,\underline{a})\hat{f}\\ =&0,\end{aligned}$$

where one has used the definition of $G_{n,m}(k,i\kappa,\underline{a})$ in Proposition 4.26. It follows that

$$R(k^2)f = \int_{\mathcal{G}} r(\cdot,y,k)\varphi(y) \in \mathrm{Dom}(T(A,B)).$$

Proof of (iii): As $\frac{i}{2k}e^{ik|x-y|}$ is the Green's function for the problem on $L^2(\mathbb{R})$, the symmetry holds for $r^0(x,y,k,ik)$ with $k \in \mathcal{Q}$. It remains to prove the symmetry of the correction term $r^1(x,y,k,ik)$. Substituting formula (62) into the formula for the correction term for appropriate k,κ gives

$$\begin{aligned}r^1(x,y,k,i\kappa) =&\Phi_{n,m}(x,k,i\kappa)(R^+_{n,m})^{-1}(k,i\kappa,\underline{a})[\mathbb{1} - \mathfrak{C}(k,i\kappa)T_{n,m}(k,i\kappa)]^{-1}\circ\\ &\circ\mathfrak{X}(k,i\kappa)(R^+_{n,m})^{-1}(k,i\kappa)J_{n,m}\Phi_{n,m}(y,k,i\kappa)^T W_{n,m}(k,i\kappa).\end{aligned}$$

Notice that $W_{n,m}$ commutes with $R^+_{n,m}$ as well as with $\Phi_{n,m}$ and $J_{n,m}$. Consider now $r(x,y,k,ik)$ for $k \in \mathcal{Q}$. Using for the diagonal matrices $I_{n,m}$ and $J_{n,m}$ the equalities

$$I^*_{n,m}J_{n,m} = I_{n,m} \quad \text{and} \quad I_{n,m}J_{n,m} = I^*_{n,m}$$

one gets

$$\begin{aligned}&\big\{[\mathbb{1} - \mathfrak{C}(k,ik)T_{n,m}(k,ik)]^{-1}\,\mathfrak{C}(k,ik)W_{n,m}(k,ik)J_{n,m}\big\}^*\\ =&\big\{[\mathbb{1} - \mathfrak{C}(k,ik)T_{n,m}(k,ik)]^{-1}\,\mathfrak{C}(k,ik)W_{n,m}(k,ik)J_{n,m}\big\}^*\\ =&J_{n,m}W_{n,m}(k,ik)^*\,\mathfrak{C}(k,ik)^*[\mathbb{1} - T_{n,m}(k,ik)^*\,\mathfrak{C}(k,ik)^*]^{-1}\\ =&\frac{i}{-2\overline{k}}I_{n,m}J_{n,m}\,\mathfrak{C}(k,ik)^*[\mathbb{1} - T_{n,m}(k,ik)^*\,\mathfrak{C}(k,ik)^*]^{-1}\\ =&\frac{i}{-2\overline{k}}[\mathbb{1} - (I^*_{n,m}\,\mathfrak{C}(k,ik)^*)I_{n,m}(T_{n,m}(k,ik)^*)]^{-1}(I^*_{n,m}\,\mathfrak{C}(k,ik)^*).\end{aligned}$$

Using the formulas given in Lemma 4.24, Chapter 4 one continues as follows

$$\begin{aligned}&\frac{i}{-2\overline{k}}[\mathbb{1} - (I^*_{n,m}\,\mathfrak{C}(k,ik)^*)I_{n,m}(T_{n,m}(k,ik)^*)]^{-1}(I^*_{n,m}\,\mathfrak{C}(k,ik)^*)\\ =&\frac{i}{-2\overline{k}}[\mathbb{1} - \mathfrak{C}(-\overline{k},i\overline{k})T_{n,m}(k,ik)^*]^{-1}\,\mathfrak{C}(-\overline{k},i\overline{k})I^*_{n,m}\\ =&[\mathbb{1} - \mathfrak{C}(-\overline{k},i\overline{k})T_{n,m}(-\overline{k},i\overline{k})]^{-1}\,\mathfrak{C}(-\overline{k},i\overline{k})W_{n,m}(-\overline{k},i\overline{k})J_{n,m}\\ =&[\mathbb{1} - \mathfrak{C}(-\overline{k},i\overline{k})T_{n,m}(-\overline{k},i\overline{k})]^{-1}\,\mathfrak{C}(-\overline{k},i\overline{k})W_{n,m}(-\overline{k},i\overline{k})J_{n,m}.\end{aligned}$$

Furthermore one has

$$R^+_{n,m}(k, ik, \underline{a})^* = R^+_{n,m}(-\overline{k}, i\overline{k}, \underline{a}) \quad \text{and} \quad \Phi(x, k, ik)^* = \Phi(x, -\overline{k}, i\overline{k}),$$

compare also [63, Proof of Lemma 4.2]. Putting the pieces together one obtains

$$r^1(k, ik, y, x)^* = r^1(-\overline{k}, i\overline{k}, x, y) \quad \text{for } k \in \mathcal{Q}$$

which proves the claim. $\square$

APPENDIX B

CONTINUATION OF THE PROOF OF PROPOSITION 4.30. The computation of the wave operators is supplemented. One computes for $k^2 = \lambda > 0$

$$\lim_{\epsilon \to 0} -i\epsilon R(k^2 \pm i\epsilon) dE_0(k) f = \lim_{\epsilon \to 0} -i\epsilon \int_{\mathcal{G}} r(x, y, \sqrt{k^2 \pm i\epsilon}) \begin{bmatrix} \cos(kx)\hat{f}_+(k) \\ 0 \end{bmatrix} dy$$

with $\{\cos(kx)\hat{f}_+(k)\}_{j\in\mathcal{E}_+} = \cos(kx_j)\hat{f}_j(k)_{j\in\mathcal{E}_+}$ and with 0 is meant the zero on the rest of the components. For $-\kappa^2 = \lambda < 0$ one computes

$$\lim_{\epsilon \to 0} -i\epsilon R(-\kappa^2 \pm i\epsilon) dE_0(\kappa) f = \lim_{\epsilon \to 0} -i\epsilon \int_{\mathcal{G}} r(x, y, \sqrt{-\kappa^2 \pm i\epsilon}) \begin{bmatrix} 0 \\ \cos(\kappa x)\hat{f}_-(\kappa) \end{bmatrix} dy$$

with $\{\cos(\kappa x)\hat{f}_-(\kappa)\}_{j\in\mathcal{E}_-} = \cos(\kappa x_j)\hat{f}_j(\kappa)_{j\in\mathcal{E}_-}$ and again 0 denotes the zero on the rest of the components.

Fix first the branch of the complex square root

$$\sqrt{\cdot}\colon \mathbb{C} \setminus [0, \infty) \to \mathbb{C}^+ \quad \text{with } \operatorname{Im} \sqrt{\cdot} > 0,$$

where $\mathbb{C}^+ = \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}$. Consider the limit values

$$\begin{aligned} k_\epsilon^+ &= \sqrt{k^2 + i\epsilon}, & k_\epsilon^- &= \sqrt{k^2 - i\epsilon}, \\ \kappa_\epsilon^+ &= \sqrt{-\kappa^2 + i\epsilon} \quad \text{and} & \kappa_\epsilon^- &= \sqrt{-\kappa^2 - i\epsilon}. \end{aligned}$$

Taking the limit $\epsilon \to 0+$ for $k > 0$ and $\kappa > 0$, respectively gives

$$\begin{aligned} \lim_{\epsilon \to 0+} k_\epsilon^+ &= k, & \lim_{\epsilon \to 0+} k_\epsilon^- &= -k, \\ \lim_{\epsilon \to 0+} \kappa_\epsilon^+ &= i\kappa \quad \text{and} & \lim_{\epsilon \to 0+} \kappa_\epsilon^- &= i\kappa. \end{aligned}$$

Observe that for $\epsilon \to 0+$ with fixed $k > 0$ and $\kappa > 0$ one has asymptotically

$$\begin{aligned} \lim_{\epsilon \to 0+} \left(\kappa_\epsilon^+ - i\kappa\right) &\sim \frac{\epsilon}{2\kappa}, & \lim_{\epsilon \to 0+} \left(\kappa_\epsilon^- - i\kappa\right) &\sim \frac{\epsilon}{2\kappa}, \\ \lim_{\epsilon \to 0+} \left(k_\epsilon^+ - k\right) &\sim \frac{i\epsilon}{2k} \quad \text{and} & \lim_{\epsilon \to 0+} \left(k_\epsilon^- + k\right) &\sim \frac{i\epsilon}{2k}. \end{aligned}$$

The following auxiliary calculations are needed,

$$
\begin{aligned}
&-i\epsilon\int_0^\infty e^{ik_\epsilon^+|x-y|}\cos(ky)dy = \\
&\frac{-i\epsilon}{2}\int_0^x e^{ik_\epsilon^+(x-y)+iky} + \frac{-i\epsilon}{2}\int_x^\infty e^{ik_\epsilon^+(y-x)+iky}dy \\
&+\frac{-i\epsilon}{2}\int_0^x e^{ik_\epsilon^+(x-y)-iky} + \frac{-i\epsilon}{2}\int_x^\infty e^{ik_\epsilon^+(y-x)-iky}dy = \\
&\frac{-i\epsilon}{2i(k-k_\epsilon^+)}e^{ik_\epsilon^+x}\left(e^{i(k-k_\epsilon^+)x}-1\right) + \frac{-i\epsilon}{2i(k_\epsilon^+ + k)}e^{-ik_\epsilon^+x}\left(-e^{i(k_\epsilon^+ + k)x}\right) \\
&+\frac{-i\epsilon}{-2i(k_\epsilon^+ + k)}e^{ik_\epsilon^+x}\left(e^{-i(k_\epsilon^+ + k)x}-1\right) + \frac{-i\epsilon}{2i(k_\epsilon^+ - k)}e^{-ik_\epsilon^+x}\left(-e^{i(k_\epsilon^+ - k)x}\right).
\end{aligned}
$$

In the limit $\epsilon \to 0+$ all summands of the right hand side except the last one vanish. The last term becomes $-ike^{-ikx}$. Consequently

$$\lim_{\epsilon\to 0+} -i\epsilon\int_0^\infty e^{ik_\epsilon^+|x-y|}\cos(ky)dy = -ike^{-ikx}.$$

Analogously one obtains

$$
\begin{aligned}
&-i\epsilon\int_0^\infty e^{ik_\epsilon^+y}\cos(ky)dy = \\
&\frac{-i\epsilon}{2}\int_0^\infty e^{ik_\epsilon^+y+iky} + \frac{-i\epsilon}{2}\int_0^\infty e^{ik_\epsilon^+y-iky}dy = \\
&\frac{-i\epsilon}{2i(k_\epsilon^+ + k)}(-1) + \frac{-i\epsilon}{2i(k_\epsilon^+ - k)}(-1).
\end{aligned}
$$

In the limit $\epsilon \to 0+$ only the second addend of the right hand side remains and takes the value $-ik$. Consequently

$$\lim_{\epsilon\to 0+} -i\epsilon\int_0^\infty e^{ik_\epsilon^+y}\cos(ky)dy = -ik.$$

Now the same calculation with k_ϵ^- yields

$$
\begin{aligned}
&-i\epsilon\int_0^\infty e^{ik_\epsilon^-|x-y|}\cos(ky)dy = \\
&\frac{-i\epsilon}{2}\int_0^x e^{ik_\epsilon^-(x-y)+iky} + \frac{-i\epsilon}{2}\int_x^\infty e^{ik_\epsilon^-(y-x)+iky}dy \\
&+\frac{-i\epsilon}{2}\int_0^x e^{ik_\epsilon^-(x-y)-iky} + \frac{-i\epsilon}{2}\int_x^\infty e^{ik_\epsilon^-(y-x)-iky}dy = \\
&\frac{-i\epsilon}{2i(k-k_\epsilon^-)}e^{ik_\epsilon^-x}\left(e^{i(k-k_\epsilon^-)x}-1\right) + \frac{-i\epsilon}{2i(k_\epsilon^- + k)}e^{-ik_\epsilon^-x}\left(-e^{i(k_\epsilon^- + k)x}\right) \\
&+\frac{-i\epsilon}{-2i(k_\epsilon^- + k)}e^{ik_\epsilon^-x}\left(e^{-i(k_\epsilon^- + k)x}-1\right) + \frac{-i\epsilon}{2i(k_\epsilon^- - k)}e^{-ik_\epsilon^-x}\left(-e^{i(k_\epsilon^- - k)x}\right).
\end{aligned}
$$

In the limit all terms on the right hand side except the second term

$$\frac{-i\epsilon}{2i(k_\epsilon^- + k)} e^{-ik_\epsilon^- x} \left(-e^{i(k_\epsilon^- + k)x} \right)$$

vanish, which becomes $-ike^{ikx}$. Consequently

$$\lim_{\epsilon \to 0+} -i\epsilon \int_0^\infty e^{ik_\epsilon^- |x-y|} \cos(ky) dy = -ike^{ikx}.$$

Analogously one obtains

$$\begin{aligned} -i\epsilon \int_0^\infty e^{ik_\epsilon^- y} \cos(ky) dy &= \frac{-i\epsilon}{2} \int_0^\infty e^{ik_\epsilon^- y + iky} + \frac{-i\epsilon}{2} \int_0^\infty e^{ik_\epsilon^- y - iky} dy \\ &= \frac{-i\epsilon}{2i(k_\epsilon^- + k)} (-1) + \frac{-i\epsilon}{2i(k_\epsilon^- - k)} (-1) . \end{aligned}$$

In the limit $\epsilon \to 0+$ only the second term remains and takes the value $-ik$. Consequently

$$\lim_{\epsilon \to 0+} -i\epsilon \int_0^\infty e^{ik_\epsilon^- y} \cos(ky) = -ik.$$

Taking into account the above auxiliary calculations yields

$$\begin{aligned} &\lim_{\epsilon \to 0+} -i\epsilon \int_{\mathcal{G}} r(x, y, \sqrt{k^2 + i\epsilon}) \begin{bmatrix} \cos(kx) \hat{f}(k) \\ 0 \end{bmatrix} dy \\ =& \lim_{\epsilon \to 0+} -i\epsilon \int_{\mathcal{G}} r^0(x, y, \sqrt{k^2 + i\epsilon}, i\sqrt{k^2 + i\epsilon}) \begin{bmatrix} \cos(kx) \hat{f}(k) \\ 0 \end{bmatrix} dy \\ +& \lim_{\epsilon \to 0+} -i\epsilon \int_{\mathcal{G}} r^1(x, y, \sqrt{k^2 + i\epsilon}, i\sqrt{k^2 + i\epsilon}) \begin{bmatrix} \cos(kx) \hat{f}(k) \\ 0 \end{bmatrix} dy \\ =& \frac{1}{2} \begin{bmatrix} e^{-ikx} \hat{f}(k) \\ 0 \end{bmatrix} + \frac{1}{2} \Phi_{n,m}(x, k, ik) G_{n,m}(k, ik) \begin{bmatrix} \hat{f}(k) \\ 0 \end{bmatrix} \\ =& \frac{1}{2} \sum_{l \in \mathcal{E}_+} \varphi_l(x, k, ik) \hat{f}_l(k). \end{aligned}$$

Analogously one obtains

$$\begin{aligned} &\lim_{\epsilon \to 0+} \int_{\mathcal{G}} r(x, y, \sqrt{k^2 - i\epsilon}) \begin{bmatrix} \cos(kx) \hat{f}(k) \\ 0 \end{bmatrix} dy \\ =& \lim_{\epsilon \to 0+} \int_{\mathcal{G}} r^0(x, y, \sqrt{k^2 - i\epsilon}, -i\sqrt{k^2 - i\epsilon}) \begin{bmatrix} \cos(kx) \hat{f}(k) \\ 0 \end{bmatrix} dy \\ +& \lim_{\epsilon \to 0+} \int_{\mathcal{G}} r^1(x, y, \sqrt{k^2 - i\epsilon}, -i\sqrt{k^2 - i\epsilon}) \begin{bmatrix} \cos(kx) \hat{f}(k) \\ 0 \end{bmatrix} dy \\ =& \frac{1}{2} \begin{bmatrix} e^{ikx} \hat{f}(k) \\ 0 \end{bmatrix} + \frac{1}{2} \Phi_{n,m}(x, -k, ik) G_{n,m}(-k, ik) \begin{bmatrix} \hat{f}(k) \\ 0 \end{bmatrix} \\ =& \frac{1}{2} \sum_{l \in \mathcal{E}_+} \varphi_l(x, -k, ik) \hat{f}_l(k). \end{aligned}$$

Using similar calculation gives

$$\lim_{\epsilon\to 0+} -i\epsilon \int_{\mathcal{G}} r(x,y,\sqrt{-\kappa^2+i\epsilon}) \begin{bmatrix} 0 \\ \cos(\kappa x)\hat{f}(\kappa) \end{bmatrix} dy = \frac{1}{2}\sum_{l\in\mathcal{E}_-} \varphi_l(x,ik,-k)\hat{f}_l(k)$$

and

$$\lim_{\epsilon\to 0+} -i\epsilon \int_{\mathcal{G}} r(x,y,\sqrt{-\kappa^2-i\epsilon}) \begin{bmatrix} 0 \\ \cos(\kappa x)\hat{f}(\kappa) \end{bmatrix} dy = \frac{1}{2}\sum_{l\in\mathcal{E}_-} \varphi_l(x,ik,k)\hat{f}_l(k).$$

Using

$$W_\pm f = \int_{-\infty}^{\infty} \lim_{\varepsilon\to 0+} -i\varepsilon R(\lambda\mp i\varepsilon)dE_0(\lambda)f,$$

one obtains that the kernel of the wave operators is given in terms of the generalized eigenfunctions. $\square$

List of Figures

List of Symbols

Bibliography

[1] Sh. Agmon. *Lectures on elliptic boundary value problems*. D. Van Nostrand Co., Inc., Princeton, N.J.-Toronto-London, 1965.

[2] S. Albeverio, F. Gesztesy, R. Høegh-Krohn and H. Holden. *Solvable models in quantum mechanics*. Texts and Monographs in Physics. Springer-Verlag, New York, 1988.

[3] G. Allaire and A. Piatnitski. Homogenization of the Schrödinger equation and effective mass theorems. *Comm. Math. Phys.*, 258(1):1–22, 2005.

[4] H. W. Alt. *Lineare Funktionalanalysis. Eine anwendungsorientierte Einführung. 2nd revisted ed.* Springer-Verlag, Berlin, 1992.

[5] W. Arendt, Ch. J. K. Batty, M. Hieber and F. Neubrander. *Vector-valued Laplace transforms and Cauchy problems*, volume 96 of *Monographs in Mathematics*. Birkhäuser Verlag, Basel, 2001.

[6] W. Arendt, R. Nittka, W. Peter and F. Steiner. Weyl's law: spectral properties of the Laplacian in mathematics and physics. In *Mathematical Analysis of Evolution, Information, and Complexity*, pages 1–71. Wiley-VCH Verlag GmbH & Co. KGaA, 2009.

[7] Y. Arlinskii, Y. Kovalev and È. R. Tsekanovskiĭ. Accretive and sectorial extensions of nonnegative symmetric operators. *Complex Analysis and Operator Theory*, 6:677–718, 2012.

[8] F. V. Atkinson and A. B. Mingarelli. Asymptotics of the number of zeros and of the eigenvalues of general weighted Sturm-Liouville problems. *J. Reine Angew. Math.*, 375/376:380–393, 1987.

[9] I. Babuška. Error-bounds for finite element method. *Numer. Math.*, 16:322–333, 1970/1971.

[10] A. Bátkai and S. Piazzera. *Semigroups for delay equations*, volume 10 of *Research Notes in Mathematics*. A K Peters Ltd., Wellesley, MA, 2005.

[11] H. Baumgärtel and M. Wollenberg. *Mathematical scattering theory*, volume 59 of *Mathematische Lehrbücher und Monographien, II. Abteilung: Mathematische Monographien*. Akademie-Verlag, Berlin, 1983.

[12] J. Behrndt and A. Luger. On the number of negative eigenvalues of the Laplacian on a metric graph. *J. Phys. A*, 43(47):474006, 11, 2010.

[13] J. Behrndt and J. Rohleder. Titchmarsh-Weyl theory for Schrödinger operators on unbounded domains. Preprint arXiv:1208.5224v1, 2012.

[14] G. Berkolaiko, R. Carlson, St. A. Fulling and P. Kuchment, editors. *Quantum graphs and their applications*, volume 415 of *Contemporary Mathematics*, American Mathematical Society, Providence, RI, 2006.

[15] P. A. Binding and H. Volkmer. Existence and asymptotics of eigenvalues of indefinite systems of Sturm-Liouville and Dirac type. *J. Differential Equations*, 172(1):116–133, 2001.

[16] P. A. Binding, D. Eschwé and H. Langer. Variational principles for real eigenvalues of self-adjoint operator pencils. *Integral Equations Operator Theory*, 38(2):190–206, 2000.

[17] M. Š. Birman and M. Z. Solomjak. Spectral asymptotics of nonsmooth elliptic operators I. *Trudy Moskov. Mat. Obšč.*, 27:3–52, 1972.

[18] J. Blank, P. Exner and M Havlíček. *Hilbert space operators in quantum physics*. Theoretical and Mathematical Physics. Springer, New York, second edition, 2008.

[19] J. Bolte and S. Endres. The trace formula for quantum graphs with general self adjoint boundary conditions. *Ann. Henri Ppropositioné*, 10(1):189–223, 2009.

[20] J. Bolte and J. Harrison. Spectral statistics for the Dirac operator on graphs. *Journal of Physics A: Mathematical and General*, 36(11):2747, 2003.

[21] A.-S. Bonnet-BenDhia, L. Chesnel A. S and P. Ciarlet. T–coercivity for scalar interface problems between dielectrics and metamaterials. *Math. Mod. Num. Anal.*, 46:1363–1387, 2012.

[22] G. Bouchitté and B. Schweizer. Cloaking of small objects by anomalous localized resonance. *Quart. J. Mech. Appl. Math.*, 63(4):437–463, 2010.

[23] T. Carleman. Propriétés asymptotiques des fonctions fondamentales des membranes vibrantes. , 1935; Collected Works, Malmö, 1960, pages 471–483.

[24] T. Carleman. Über die asymptotische Verteilung der Eigenwerte partieller Differentialgleichungen. *Ber. Sächs. Akad. Wiss. Leipzig, math.-phys. Kl.*, 88:119–132, 1936; Collected Works, Malmö, 1960, pages 483–497.

[25] B. Ćurgus and B. Najman. The operator $(\operatorname{sgn} x)d^2/dx^2$ is similar to a selfadjoint operator in $L^2(\mathbf{R})$. *Proc. Amer. Math. Soc.*, 123(4):1125–1128, 1995.

[26] S. Currie and B. A. Watson. Indefinite boundary value problems on graphs. *Oper. Matrices*, 5(4):565–584, 2011.

[27] S. Datta. *Quantum Transport - Atom to Transistor*. Cambridge University Press, 2005.

[28] R. Dautray and J.-L. Lions. *Mathematical analysis and numerical methods for science and technology. Vol. 3*. Springer-Verlag, Berlin, 1990.

[29] E. B. Davies, P. Exner and J. Lipovský. Non-Weyl asymptotics for quantum graphs with general coupling conditions. *J. Phys. A*, 43(47):474013, 16, 2010.

[30] V. A. Derkach, M. M. Malamud and È. R. Tsekanovskiĭ. Sectorial extensions of a positive operator, and the characteristic function. *Ukrain. Mat. Zh.*, 41(2):151–158, 286, 1989.

[31] D. P. DiVincenzo and E. J. Mele. Self-consistent effective-mass theory for intralayer screening in graphite intercalation compounds. *Phys. Rev. B*, 29(4):1685–1694, 1984.

[32] N. Dunford and J. T. Schwartz. *Linear operators. Part III: Spectral operators*. Pure and Applied Mathematics, Vol. VII. Interscience Publishers, New York-London-Sydney, 1971.

[33] K.-J. Engel and R. Nagel. *One-parameter semigroups for linear evolution equations*, volume 194 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 2000.

[34] D. Eschwé and M. Langer. Variational principles for eigenvalues of self-adjoint operator functions. *Integral Equations Operator Theory*, 49(3):287–321, 2004.

[35] P. Exner. Momentum operators on graphs. Preprint arXiv:1205.5941 (to appear in Fritz Gesztesy Festschrift), 2012.

[36] P. Exner and O. Post. Convergence of spectra of graph-like thin manifolds. *J. Geom. Phys.*, 54(1):77–115, 2005.

[37] W. G. Faris. *Self-adjoint operators*. Lecture Notes in Mathematics, Vol. 433. Springer-Verlag, Berlin, 1975.

[38] A. Fleige, S. Hassi and H. de Snoo. A Kreĭn space approach to representation theorems and generalized Friedrichs extensions. *Acta Sci. Math. (Szeged)*, 66(3-4):633–650, 2000.

[39] F. Gastaldi and A. Quarteroni. On the coupling of hyperbolic and parabolic systems: analytical and numerical approach. In *Applications of mathematics in industry and technology (Siena, 1988)*, pages 123–165. Teubner, Stuttgart, 1989.

[40] I. C. Gohberg and M. G. Kreĭn. *Introduction to the theory of linear nonselfadjoint operators*. Translations of Mathematical Monographs, Vol. 18. American Mathematical Society, Providence, R.I., 1969.

[41] D. Grieser. Spectra of graph neighborhoods and scattering. *Proc. Lond. Math. Soc. (3)*, 97(3):718–752, 2008.

[42] P. Grisvard. *Elliptic problems in nonsmooth domains*, volume 24 of *Monographs and Studies in Mathematics*. Pitman (Advanced Publishing Program), Boston, MA, 1985.

[43] L. Grubišić, V. Kostrykin, K. A. Makarov and K. Veselić. Representation theorems for indefinite quadratic forms revisited. *Mathematika* (to appear), Preprint arXiv:1003.1908, 2010.

[44] L. Guillopé. Sur la théorie spectral de quelques variétés non compactes. *Séminaire de théorie spectrale et géométrie*, pages 115–126, 1985-86.

[45] L. Guillopé. Théorie spectrale de quelques variétés à bouts. *Ann. Sci. École Norm. Sup. (4)*, 22(1):137–160, 1989.

[46] K. E. Gustafson and D. K. M. Rao. *Numerical range*. Universitext. Springer-Verlag, New York, 1997.

[47] M. Harmer. Hermitian symplectic geometry and extension theory. *J. Phys. A*, 33(50):9193–9203, 2000.

[48] J. Hou. On the spectra of the positive completions for operator matrices. *J. Operator Theory*, 33(2):299–315, 1995.

[49] A. Hurwitz. Ueber die angenäherte Darstellung der Irrationalzahlen durch rationale Brüche. *Mathematische Annalen*, 39:279–284, 1891.

[50] A. Hussein. Zur Streutheorie von Diracoperatoren. *Diplomarbeit*, Rheinische Friedrich Wilhelms Universität, Bonn, 2008.

[51] A. Hussein. Maximal–quasi–accretive Laplacians on finite metric graphs. Preprint arXiv:1211.4143v2, 2012.

[52] A. Hussein. Sign–indefinite second order differential operators on finite metric graphs. Preprint arXiv:1211.4144v2, 2012.

[53] A. Hussein. Bounds on the negative eigenvalues of laplacians on finite metric graphs. *Integral Equations and Operator Theory*, 76(3):381–401, 2013.

[54] A. Hussein and D. Mugnolo. Quantum graphs with mixed dynamics: the transport/diffusion case. *J. Phys. A: Math. Theor.*, 46(23):235202, 2013.

[55] Kh. Hussein. *Palästinensische Studentinnen an israelischen Hochschulen*. PhD thesis, Carl von Ossietzky Universität Oldenburg, 2006.

[56] A. Hussein, V. Kostrykin, D. Krejčiřík and St. Schmitz. In preparation.

[57] V. Ivrii. *Microlocal analysis and precise spectral asymptotics*. Springer Monographs in Mathematics. Springer-Verlag, Berlin, 1998.

[58] T. Kato. *Perturbation theory for linear operators*. Die Grundlehren der mathematischen Wissenschaften, Band 132. Springer-Verlag New York, Inc., New York, 1966.

[59] A. N. Kočubeĭ. Extensions of symmetric operators and of symmetric binary relations. *Mat. Zametki*, 17:41–48, 1975.

[60] V. Kostrykin and R. Schrader. Kirchhoff's rule for quantum wires. *J. Phys. A*, 32(4):595–630, 1999.

[61] V. Kostrykin and R. Schrader. The generalized star product and the factorization of scattering matrices on graphs. *J. Math. Phys.*, 42(4):1563–1598, 2001.

[62] V. Kostrykin and R. Schrader. The inverse scattering problem for metric graphs and the traveling salesman problem. Preprint arXiv:math-ph/0603010v1, 2006.

[63] V. Kostrykin and R. Schrader. Laplacians on metric graphs: eigenvalues, resolvents and semigroups. In *Quantum graphs and their applications*, volume 415 of *Contemp. Math.*, pages 201–225. Amer. Math. Soc., Providence, RI, 2006.

[64] V. Kostrykin, J. Potthoff and R. Schrader. Heat kernels on metric graphs and a trace formula. In *Adventures in mathematical physics*, volume 447 of *Contemp. Math.*, pages 175–198. Amer. Math. Soc., Providence, RI, 2007.

[65] V. Kostrykin, J. Potthoff and R. Schrader. Brownian motions on metric graphs: Feller Brownian motions on intervals revisited. Preprint arXiv:1008.3761v2, 2010.

[66] V. Kostrykin, J. Potthoff and R. Schrader. Brownian motions on metric graphs I - Definition, Feller property, and generators. Preprint arXiv:1008.3761v2, 2010.

[67] V. Kostrykin, J. Potthoff and R. Schrader. Brownian motions on metric graphs II - Construction of Brownian motions on single vertex graphs. Preprint arXiv:1008.3761v2, 2010.

[68] V. Kostrykin, J. Potthoff and R. Schrader. Brownian motions on metric graphs III - Construction: General metric graphs. Preprint arXiv:1008.3761v2, 2010.

[69] M. Kramar and E. Sikolya. Spectral properties and asymptotic periodicity of flows in networks. *Math. Z.*, 249(1):139–162, 2005.

[70] D. Krejčiřík and H. Šediváková. The effective Hamiltonian in curved quantum waveguides under mild regularity assumptions. *Reviews in Mathematical Physics*, 24(07):1250018, 2012.

[71] P. Kuchment. Graph models for waves in thin structures. *Waves Random Media*, 12(4):R1–R24, 2002.

[72] P. Kuchment. Quantum graphs. I. Some basic structures. *Waves Random Media*, 14(1):S107–S128, 2004.

[73] O. A. Ladyzhenskaya. *The boundary value problems of mathematical physics*, volume 49 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1985.

[74] M. M. Malamud. Some classes of extensions of a Hermitian operator with lacunae. *Ukraïn. Mat. Zh.*, 44(2):215–233, 1992.

[75] A. G. R. McIntosh. Bilinear forms in Hilbert space. *J. Math. Mech.*, 19:1027–1045, 1969/1970.

[76] J. Nečas. *Les méthodes directes en théorie des équations elliptiques*. Masson et Cie, Éditeurs, Paris, 1967.

[77] D. S. Novikov. Scattering theory and transport in graphene. Preprint arXiv:0706.1391, 2007.

[78] R. G. Novikov. Formulae and equations for finding scattering data from the Dirichlet-to-Neumann map with nonzero background potential. *Inverse Problems*, 21(1):257, 2005.

[79] A. Pazy. *Semigroups of linear operators and applications to partial differential equations*, volume 44 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1983.

[80] O. Post. First order approach and index theorems for discrete and metric graphs. *Annales Henri Poincaré*, 10(5):823–866, 2009.

[81] R. Redheffer. Difference equations and functional equations in transmission-line theory. In *Modern mathematics for the engineer: Second series*, pages 282–337. McGraw-Hill, New York, 1961.

[82] R. Redheffer. On the relation of transmission-line theory to scattering and transfer. *J. Math. and Phys.*, 41:1–41, 1962.

[83] M. Reed and B. Simon. *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*. Academic Press, New York, 1975.

[84] A. Scott. *Neuroscience*. Springer-Verlag, New York, 2002.

[85] P. Siegl. Surprising spectra of PT-symmetric point interactions. Preprint arXiv:0906.0226, 2009.

[86] D. R. Smith, J. B. Pendry, and M. C. K. Wiltshire. Metamaterials and negative refractive index. *Science*, 305:788–92, 2004.

[87] H. Sohr. *The Navier-Stokes equations*. Birkhäuser Advanced Texts: Basler Lehrbücher. Birkhäuser Verlag, Basel, 2001.

[88] Ch. Tretter. *Spectral theory of block operator matrices and applications*. Imperial College Press, London, 2008.

[89] È. R. Tsekanovskiĭ. Accretive extensions and problems on the Stieltjes operator-valued functions relations. In *Operator theory and complex analysis (Sapporo, 1991)*, volume 59 of *Oper. Theory Adv. Appl.*, pages 328–347. Birkhäuser, Basel, 1992.

[90] V. G. Veselago. The electrodynamics of substances with simultaneously negative values of ϵ and μ. *Sov. Phys. Usp.*, 10(4):509–514, 1968.

[91] J. Weidmann. *Spectral theory of ordinary differential operators*, volume 1258 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1987.

[92] J. Weidmann. *Lineare Operatoren in Hilberträumen. Teil 1*. Mathematische Leitfäden. Teubner, Stuttgart, 2000.

[93] J. Weidmann. *Lineare Operatoren in Hilberträumen. Teil II*. Mathematische Leitfäden. Teubner, Stuttgart, 2003.

[94] H. Weyl. Das asymptotische Verteilungsgesetz der Eigenwerte linearer partieller Differentialgleichungen (mit einer Anwendung auf die Theorie der Hohlraumstrahlung). *Math. Ann.*, 71(4):441–479, 1912.

[95] D.N. Wheatley. Diffusion theory, the cell and the synapse. *Biosystems*, 45(2):151 – 163, 1998.

[96] D. R. Yafaev. *Mathematical scattering theory*, volume 158 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2010.

[97] A. Zettl. *Sturm-Liouville theory*, volume 121 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2005.

[98] F. Zhang, editor. *The Schur complement and its applications*, volume 4 of *Numerical Methods and Algorithms*. Springer-Verlag, New York, 2005.

[99] Y. Zhang, Y.-W. Tan, H. L. Stormer and Ph. Kim. Experimental observation of the quantum Hall effect and Berry's phase in graphene. *Nature*, 438:201–204, November 2005.

[100] M. Znojil and G. Lévai. Schroedinger equations with indefinite effective mass. *Physics Letters A*, 376(45):3000–3005, 2012.