



# SJÄLVSTÄNDIGA ARBETEN I MATEMATIK

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## Faber-Krahn inequalities for point-interaction Hamiltonians in bounded domains

av

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### **Abstract**

This thesis concerns the minimization of the lowest eigenvalue of certain perturbations of the Dirichlet Laplacian on a bounded domain with potential supported on a discrete set of points. Recent results include a Faber-Krahn-type inequality, valid when the support is a single point. We show that some of the methods used to prove this inequality can be generalized to an abstract operator-theoretic setting, and we use this to obtain a new Faber-Krahn-type inequality for when the support consists of more than one point. Our approach also yields some additional results on the lowest eigenvalue, such as it being simple.

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# 1 Introduction

## 1.1 Background

Let  $\Omega$  be a bounded open subset of  $\mathbb{R}^d$ ,  $d \geq 1$ . The negative Laplacian (henceforth just “Laplacian”) is the linear partial differential expression

$$-\Delta := -\sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}$$

and appears in many different mathematical and physical contexts, not least due to the ubiquity of Laplace’s equation

$$-\Delta f = 0 \quad \text{on } \Omega$$

which describes a wide array of natural phenomena. For example, Fick’s law of diffusion, Fourier’s law of heat conduction, and Ohm’s law of electrical conduction are all special cases of Laplace’s equation [10]. On the other hand, a math major’s first encounter with the Laplacian might typically be an undergraduate course on complex analysis, in which the real and imaginary parts of functions holomorphic on  $\Omega$  are seen to solve Laplace’s equation, and the second encounter might follow in a course on partial differential equations, where the Laplacian in addition to being studied in and of itself also proves useful in understanding the wave and heat equations [10]. For more discussion of the ubiquity of Laplace’s equation in mathematical physics, see [13, Chapter 12].

Especially important is the Dirichlet eigenvalue problem on  $\Omega$ , which is to find those real numbers  $\lambda$  (“eigenvalues”) for which there exists a nonzero function  $f$  (an “eigenfunction” corresponding to  $\lambda$ ) such that

$$\begin{cases} -\Delta f = \lambda f & \text{on } \Omega, \\ f = 0 & \text{on } \partial\Omega. \end{cases} \quad (1)$$

Whereas the classical formulation of (1) requires  $f \in C^2(\Omega) \cap C(\overline{\Omega})$ , the modern approach is instead to encode the boundary condition by letting  $-\Delta$  act on a carefully chosen subspace of the Hilbert space  $L^2(\Omega)$  of square-integrable functions on  $\Omega$ , which allows for much “rougher” eigenfunctions that may not even be pointwise defined on  $\partial\Omega$ . This gives rise to a realization of the Laplacian as an unbounded self-adjoint operator  $-\Delta_D^\Omega$  in  $L^2(\Omega)$  [28, Section 10.6]. From this point of view, solving (1) becomes equivalent to finding those  $\lambda$  such that the operator  $-\Delta_D^\Omega - \lambda$  has nontrivial kernel. The set of all such  $\lambda$  is then called the spectrum of the operator  $-\Delta_D^\Omega$ .

One can show that the spectrum of  $-\Delta_D^\Omega$  is countably infinite and that its points can be arranged in an increasing sequence  $0 < \lambda_1(\Omega) < \lambda_2(\Omega) < \dots$  such that  $\lambda_n(\Omega) \rightarrow \infty$  as  $n \rightarrow \infty$  [18, Theorem 1.2.2]. The lowest eigenvalue  $\lambda_1(\Omega)$  is called the principal (Dirichlet) eigenvalue. In the context of the wave equation on  $\Omega$ , finding the standing waves reduces to solving (1), and this leads

in the one- or two-dimensional case to a physical interpretation of  $\lambda_1(\Omega)$  as the fundamental frequency of either a vibrating string with fixed endpoints (in dimension one) or a vibrating drum with fixed edge (in dimension two), while the other eigenvalues correspond to the overtones [6].

As every musician knows—though some perhaps only subconsciously—the distribution of the overtones is an important factor in the timbre of a tone, and is to some extent what allows a listener to distinguish between notes of the same pitch when performed by different musical instruments [29]. The possibility of inferring the shape of an instrument from its overtones was pondered by M. Kac in a 1966 lecture titled *Can one hear the shape of a drum?* [21] where he asked: If  $\Omega_1$  and  $\Omega_2$  are two bounded domains in the plane such that  $\lambda_n(\Omega_1) = \lambda_n(\Omega_2)$  for all  $n \geq 1$ , is it necessarily the case that  $\Omega_1$  and  $\Omega_2$  are congruent? His question was later answered in the negative by C. Gordon, D. Webb, and S. Wolpert in an article succinctly titled *One cannot hear the shape of a drum* [16], in which they constructed a counterexample.

Arguably the first problem in this direction was posed already in 1877, when Lord Rayleigh published his book “The theory of sound” [25] in which he conjectured, based on computations and physical evidence, that “...among all drums of the same area and the same tension the circular drum produces the lowest fundamental frequency” [6]. He was proven right nearly six decades later when G. Faber [12] and E. Krahn [23] simultaneously and independently proved what is now known as the Faber-Krahn inequality, which in its modern formulation asserts that

$$\lambda_1(B) \leq \lambda_1(\Omega) \tag{2}$$

for any open ball  $B \subset \mathbb{R}^d$  with the same volume (Lebesgue measure) as  $\Omega$  [18, Theorem 3.2.1]. Under some additional regularity assumptions on the allowable domains  $\Omega$ , one can also show that the ball is also the unique minimizer.

The study of the interplay between geometry and spectrum grew over the next century into a field aptly named spectral geometry. In fact, for some natural classes of  $\Omega$ , even the original problem of minimizing  $\lambda_1(\Omega)$  is far from settled: we refer to [18, Chapter 3] for a few easy-to-formulate yet open problems, one of which is to prove that “...the regular  $N$ -gone has the least first eigenvalue among all the  $N$ -gones of given area for  $N \geq 5$ .” The setting has also been successfully generalized from Euclidean domains to domains in Riemannian manifolds; see, e.g., [9, Chapter IV].

After its debut in the 1920s, the Faber-Krahn inequality has since been extended to many other settings; see [6, Chapter 4] for a survey. The extension most relevant for this thesis is to Schrödinger operators, i.e., perturbations of the Laplacian of the form

$$H_V := -\Delta + V \tag{3}$$

where  $V \in L^1(\Omega)$  is a potential. More precisely, assuming  $V$  is nonnegative and letting  $\lambda_1(\Omega, V)$  denote the principal eigenvalue of  $H_V$ , one can use the symmetric decreasing rearrangement (see the appendix) to prove the Faber-Krahn-type inequality

$$\lambda_1(\Omega^*, V^*) \leq \lambda_1(\Omega, V) \tag{4}$$

where  $\Omega^*$  (resp.  $V^*$ ) denotes the symmetric decreasing rearrangement of  $\Omega$  (resp.  $V$ ) [6, Theorem 4.2]. Taking  $V \equiv 0$  in (4) yields the original Faber-Krahn inequality, which is typical of such generalizations. Schrödinger operators are also highly relevant for our next topic: point-interaction Hamiltonians.

In nonrelativistic quantum mechanics, each physical system has an associated complex Hilbert space, its state space  $\mathcal{H}$ , such that at any instance of time the state of the system is described by a unit vector in  $\mathcal{H}$ . Until a measurement is performed on the system, its time evolution  $\psi(t) \in \mathcal{H}$  is deterministic and obeys the Schrödinger equation

$$i\hbar \frac{d}{dt} \psi(t) = H\psi(t),$$

where  $i$  is the imaginary unit,  $\hbar$  is the reduced Planck's constant, and  $H$  is a self-adjoint operator in  $\mathcal{H}$  called the Hamiltonian [30, Section 5.1].

As for  $-\Delta_D^\Omega$  we define the eigenvalues of  $H$  as those  $\lambda$  such that  $H - \lambda$  has nontrivial kernel, but a new addition is that the spectrum of  $H$  already comes equipped with a physical interpretation, namely as the set of possible energy levels of the system. Upon measuring the energy we will observe one of these energy levels  $\lambda$ , and, according to the postulates of quantum mechanics, the system will then immediately enter a state described by a normalized eigenfunction of  $H$  corresponding to  $\lambda$  [30, Section 5.4].

Each physical system has its own Hamiltonian. For example, to model a free particle with mass  $m$  in  $\mathbb{R}^d$ ,  $d \leq 3$  we use the state space  $\mathcal{H} = L^2(\mathbb{R}^d)$  and Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m} \Delta, \tag{5}$$

where again  $-\Delta$  acts on some carefully chosen subspace of  $L^2(\mathbb{R}^d)$  so as to make  $H$  self-adjoint [30, Section 6.1]. With the same state space, an electron with mass  $\mu$  and negative charge  $-e$  orbiting a proton can instead be modeled using the Hamiltonian

$$H_e = -\frac{\hbar^2}{2\mu} \Delta + V_e$$

where  $V_e(x) = -e^2/|x|$  is the Coulomb potential [30, Chapter 9]. This Hamiltonian is of the form (3) and therefore an example of a Schrödinger operator.

If instead we desire to model a particle with mass  $m$  “subject to a very intense force with a range much shorter than the wavelength associated to the particle,” then a point-interaction Hamiltonian is appropriate [30, Section 8.1]. Formally and in one dimension, such Hamiltonians have the form

$$H_\nu = -\frac{\hbar^2}{2m} \Delta + \nu \delta_y,$$

where  $y \in \mathbb{R}$  is the interaction center,  $\delta_y$  is a delta distribution, and  $\nu \in \mathbb{R}$  is “a coupling constant which represents the strength of the interaction.” The intuition of an intense but short-ranged force is supported by the fact that  $H_\nu$  may be constructed as a suitable limit of Schrödinger operators  $H_V$  where

the potential  $V$  shrinks and spikes up to a delta-like profile [2]. In practice, however,  $H_\nu$  is constructed by restricting (5) to a set of functions vanishing at  $y$  and then carefully extending this restriction so as to obtain a self-adjoint operator different from (5).

Point-interaction Hamiltonians with multiple interaction centers in  $\mathbb{R}^d$ ,  $d \leq 3$  have been extensively studied (see, e.g., [1, 3]), to the extent that the corresponding quantum-mechanical models are considered solvable “...in the sense that their resolvents and associated mathematical and physical quantities like the spectrum, the corresponding eigenfunctions, resonances, and scattering quantities can be determined explicitly” [1]. Such Hamiltonians can then for example be used to describe “...the motion of a quantum mechanical particle moving under the action of a potential supported, e.g., by the points of a crystal lattice or a random solid” [3].

More recently, in 2007, Blanchard et al. [8] used the self-adjoint extension theory of boundary triplets to construct point-interaction Hamiltonians with multiple interaction centers confined in bounded domains. Particular attention was paid to the case of a single interaction center, and later investigations such as [11] kept this line of inquiry by investigating the optimization of the principal eigenvalue of such Hamiltonians with respect to the domain and placement of center. It was in this context that Lotoreichik and Michelangeli [24] in 2020 derived an analogue of the Faber-Krahn-type inequality (4) for potentials supported at a single point. More specifically, they proved that for any two- or three-dimensional smooth bounded domain  $\Omega$  and any  $y \in \Omega$ ,

$$\lambda_1^\alpha(B, 0) \leq \lambda_1^\alpha(\Omega, y) \quad \text{for all } \alpha \in \mathbb{R}, \quad (6)$$

where  $\lambda_1^\alpha(\Omega, y)$  is the principal eigenvalue of the point-interaction Hamiltonian in  $\Omega$  with interaction center at  $y$  and extension parameter  $\alpha$ , and  $B$  is the open ball centered at the origin with the same volume as  $\Omega$  [24, Theorem 5.1]. (The parameter  $\alpha$  has a physical interpretation as the “inverse scattering length”.)

It was with this background that the author set out to attempt to generalize (6) to the multi-point case.

## 1.2 Outline and summary of results

In Section 2, we present the reader with most of the mathematical tools needed to understand this thesis. Propositions are either proved or cited as necessary, and we provide additional references for further reading.

In Section 3, after introducing some additional tools we present our first results. These are abstract and operator-theoretic in nature: We define and study triplets  $(T, \mathbb{E}, \mathbf{W})$  consisting of

1. a densely defined lower semibounded symmetric operator  $T$  in a Hilbert space with finite defect indices  $(m, m)$ ,
2. a family  $\mathbb{E} = \{\mathbb{E}_\lambda : \lambda < \mathfrak{m}(T)\}$  of bases of defect spaces of  $T$  that are in a certain sense compatible with each other, and

3. a family  $\mathbf{W} = \{\mathbf{W}(\lambda) : \lambda < \mathfrak{m}(T)\}$  of Hermitian  $m \times m$  matrices that is in a certain sense compatible with  $\mathbb{E}$ .

We prove an extension theorem (Theorem 3.43) that uses the data in  $(T, \mathbb{E}, \mathbf{W})$  to parametrize some of the self-adjoint extensions of  $T$  by Hermitian matrices. The theorem furnishes explicit formulas for the domain, action, and quadratic form of the extension, and these formulas include an additional real parameter that can be varied to obtain different representations. We then prove a key result (Theorem 3.44) asserting that for any parameter  $\mathbf{B}$ , the principal eigenvalue of the corresponding extension  $T_{\mathbf{B}}$  is controlled by  $\mathbf{W}$  in the sense that

$$\mathfrak{m}(T_{\mathbf{B}}) = \lambda \quad \text{if and only if} \quad \lambda_{\max}(\mathbf{W}(\lambda) - \mathbf{B}) = 0.$$

We also study the case  $m = 1$  in more detail (Section 3.7).

Next we require some notation. Let  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$  be a bounded domain with  $C^\infty$ -boundary, let  $X = \{x_1, \dots, x_m\} \subset \Omega$ , and let  $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{R}^m$ . Let  $\lambda_1(\Omega, X, \alpha)$  be the principal eigenvalue of the point-interaction Hamiltonian in  $\Omega$  with interaction centers  $X$  such that  $x_i$  has interaction parameter  $\alpha_i$  for each  $i = 1, \dots, m$  (as defined in [8, Section III]).

In Section 4, we apply the theory of Section 3 to construct the aforementioned Hamiltonians in a novel way (Section 4.4). In addition, we prove a few results for which it is difficult to find explicit references in the literature: We show that  $\lambda_1(\Omega, X, \alpha)$  is a simple eigenvalue (Theorem 4.39), that  $\alpha_i \mapsto \lambda_1(\Omega, X, \alpha)$  is analytic and strictly increasing for each  $i = 1, \dots, m$  (also Theorem 4.39), and that if a new interaction center  $x_{m+1}$  with new parameter  $\alpha_{m+1}$  is added to  $X$  while the old parameters  $\alpha_1, \dots, \alpha_m$  are kept the same, then  $\lambda_1(\Omega, X, \alpha)$  decreases (Theorem 4.41).

In Section 5, we turn to the subject of Faber-Krahn-type inequalities. We first prove a general operator-theoretic result (Theorem 5.3) that allows us to efficiently recover (6) and which we believe could potentially be used to derive inequalities similar to (6) in other settings. Our main result (Theorem 5.8) is a novel Faber-Krahn-type inequality in the likeness of (6) and states: If  $m \geq 2$ , then there exist positive constants  $G_1, \dots, G_m$  only dependent on  $\Omega$  and  $X$  such that

$$\lambda_1(B, \{0\}, \min_{1 \leq i \leq m} \{\alpha_i - G_i\}) \leq \lambda_1(\Omega, X, \alpha)$$

for all  $\alpha \in \mathbb{R}^m$  such that  $\lambda_1(\Omega, X, \alpha) \leq 0$ . Finally, we argue that one of the proof strategies employed by [24] fails in the multi-point case (Section 5.4).

## 2 Preliminaries

In this section we recall some basic definitions and results from the spectral theory of (unbounded) linear operators in Hilbert space with the purpose of making this thesis as self-contained as possible. We will restrict our attention to spaces defined over the complex numbers, but the reader should note that much of the theory holds also when the scalars are the real numbers.

As additional references we suggest the following books: [14] provides a good introduction to measure and Lebesgue integration theory, functional analysis,  $L^2$ -spaces, and some elementary Banach and Hilbert space theory. Two comprehensive references for the theory of linear operators in Hilbert space and their spectral theory are [31] and [28], where the former includes a more detailed treatment of Hilbert spaces, whilst the latter is newer and contains some material on sesquilinear forms and self-adjoint extension theory that the former does not.

## 2.1 Normed spaces and Banach spaces

Let  $V$  be a vector space over  $\mathbb{C}$ . A *norm* on  $V$  is a map  $\|\cdot\| : V \rightarrow \mathbb{C}$  such that

- (i)  $\|u\| \geq 0$  for all  $u \in V$ , with equality if and only if  $u = 0$ ;
- (ii)  $\|au\| = |a| \|u\|$  for all  $a \in \mathbb{C}$ ,  $u \in V$ ;
- (iii) the *triangle inequality* holds:  $\|u + v\| \leq \|u\| + \|v\|$  for all  $u, v \in V$ .

A *normed space* is a pair  $(V, \|\cdot\|)$  as above, but by a slight abuse of notation we usually refer to  $V$  itself as the normed space.

Any norm on  $V$  induces a metric on  $V$  by  $d(u, v) := \|u - v\|$ , which in turn induces a topology on  $V$ . When we hereafter speak of topological properties such as closedness or compactness of subsets of  $V$  we always mean with respect to this induced topology. We say that the normed space  $V$  is a *Banach space* if  $V$  is complete as a metric space with respect to the induced metric.

## 2.2 Bounded operators and compact operators

Let  $V, W$  be normed spaces and let  $T : V \rightarrow W$  be a linear operator (i.e., a linear map). We say that  $T$  is *bounded* if there exists a nonnegative constant  $C$  such that

$$\|Tu\| \leq C \|u\| \quad \text{for all } u \in V.$$

The least upper bound of all such  $C$  is denoted  $\|T\|$ , and it too has the property that

$$\|Tu\| \leq \|T\| \|u\| \quad \text{for all } u \in V.$$

The set of all bounded linear operators  $V \rightarrow W$  is denoted  $\mathcal{B}(V, W)$ , and is a normed space with norm  $T \mapsto \|T\|$ . This norm is called the *operator norm*, or sometimes the *uniform norm*. If  $W$  is a Banach space, then  $\mathcal{B}(V, W)$  is a Banach space with respect to the operator norm [31, Theorem 4.6]. If  $W = V$ , then we just write  $\mathcal{B}(V) := \mathcal{B}(V, V)$ .

We say that the linear operator  $T : V \rightarrow W$  is *compact* if  $T$  maps bounded subsets of  $V$  onto relatively compact subsets of  $W$ . One can show that every compact operator is bounded [31, Theorem 6.2].

## 2.3 Inner product spaces and Hilbert spaces

Let  $V$  be a vector space over  $\mathbb{C}$ . An *inner product* on  $V$  is a map  $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{C}$  such that

- (i)  $u \mapsto \langle u, v \rangle$  is linear for each fixed  $v \in V$ ;
- (ii)  $\langle u, v \rangle = \overline{\langle v, u \rangle}$  for all  $u, v \in V$ ;
- (iii)  $\langle u, u \rangle \geq 0$  for all  $u \in V$ , with equality if and only if  $u = 0$ .

(i) and (ii) together imply that  $v \mapsto \langle u, v \rangle$  is antilinear for each fixed  $u \in V$ . An *inner product space* is a pair  $(V, \langle \cdot, \cdot \rangle)$  as above, but by a slight abuse of notation we usually refer to  $V$  itself as the inner product space.

Any inner product on  $V$  induces a norm on  $V$  by  $\|u\| := \sqrt{\langle u, u \rangle}$ , which in turn induces a topology. The *Cauchy-Schwarz inequality* [31, Theorem 1.4] says that

$$|\langle u, v \rangle| \leq \|u\| \|v\| \quad \text{for all } u, v \in V.$$

As a consequence of the Cauchy-Schwarz inequality, we find [31, Section 2.1] that the maps  $u \mapsto \langle u, v \rangle$  and  $v \mapsto \langle u, v \rangle$  (resp.  $(u, v) \mapsto \langle u, v \rangle$ ) are continuous with respect to the induced topology of  $V$  (resp.  $V \times V$ ). We say that the inner product space  $V$  is a *Hilbert space* if it is a Banach space with respect to the induced norm.

Let  $V$  be an inner product space. The *orthogonal complement* of a subset  $A \subset V$  is the set

$$A^\perp := \{u \in V : \langle u, v \rangle = 0 \text{ for all } v \in A\}.$$

One can show the following [31, Section 3.1]:  $A^\perp$  is a closed subspace of  $V$ , and if  $V$  is a Hilbert space, then  $A^{\perp\perp} = \overline{\text{span } A}$ . In addition, if  $V$  is a Hilbert space and  $A$  is a subspace, then  $A$  is dense in  $V$  if and only if  $A^\perp = \{0\}$ .

Let  $(V_i, \langle \cdot, \cdot \rangle_i)$ ,  $i = 1, 2$  be two inner product spaces. The Cartesian product  $V_1 \times V_2$  of the underlying vector spaces is itself a vector space under component-wise vector addition and scalar multiplication. Moreover,

$$\langle (u_1, u_2), (v_1, v_2) \rangle := \langle u_1, v_1 \rangle_1 + \langle u_2, v_2 \rangle_2 \quad \text{for } (u_1, u_2), (v_1, v_2) \in V_1 \times V_2$$

defines an inner product on  $V_1 \times V_2$ . The resulting inner product space is called the *direct sum* of  $V_1$  and  $V_2$  and is usually denoted  $V_1 \oplus V_2$ . If in addition both  $V_1$  and  $V_2$  are Hilbert spaces, then  $V_1 \oplus V_2$  is also a Hilbert space.

## 2.4 Linear operators on Hilbert spaces

Let  $\mathcal{H}$  be a Hilbert space. A *linear operator* (or just “operator”) in  $\mathcal{H}$  is a linear operator  $T : \mathcal{D}(T) \rightarrow \mathcal{H}$ , where  $\mathcal{D}(T)$  is a linear subspace of  $\mathcal{H}$ .  $\mathcal{D}(T)$  is called the *domain* of  $T$ , and we say that the operator  $T$  is *everywhere defined* (resp. *densely defined*) if  $\mathcal{D}(T) = \mathcal{H}$  (resp.  $\mathcal{D}(T)$  is dense in  $\mathcal{H}$ ). The *kernel/nullspace* of  $T$  is the subspace  $\mathcal{N}(T) = \{f \in \mathcal{D}(T) : Tf = 0\}$ , and the *range/image* of

$T$  is the subspace  $\mathcal{R}(T) = \{Tf : f \in \mathcal{D}(T)\}$ . We say that  $T$  is *injective* if  $\mathcal{N}(T) = \{0\}$ , and in this case we define its *inverse*  $T^{-1}$  as the operator in  $\mathcal{H}$  having domain  $\mathcal{D}(T^{-1}) = \mathcal{R}(T)$  and action  $T^{-1}f := g$ , where  $g$  is the unique  $g \in \mathcal{D}(T)$  such that  $f = Tg$ .

We say that a linear operator  $T$  in  $\mathcal{H}$  is *bounded* (resp. *compact*) if the linear operator  $T : \mathcal{D}(T) \rightarrow \mathcal{H}$  is bounded (resp. compact) with respect to the norm induced by the inner product of  $\mathcal{H}$ .

The everywhere defined identity map on  $\mathcal{H}$  will be denoted by  $I$ , and, for any  $z \in \mathbb{C}$ , the everywhere defined scalar multiplication map  $f \mapsto zf$  on  $\mathcal{H}$  will by a slight abuse of notation be denoted by  $z$ .

Let  $T$  be a linear operator in  $\mathcal{H}$ . Its domain  $\mathcal{D}(T)$  is an inner product space with inner product

$$\langle f, g \rangle_T := \langle f, g \rangle + \langle Tf, Tg \rangle \quad \text{for } f, g \in \mathcal{D}(T),$$

and the corresponding induced norm  $\|f\|_T := \sqrt{\langle f, f \rangle_T}$  is called the *graph norm* of  $T$ . We say that  $T$  is *closed* if  $(\mathcal{D}(T), \langle \cdot, \cdot \rangle_T)$  is a Hilbert space. One can show that if  $T$  is closed, then  $\mathcal{N}(T)$  is a closed subspace of  $\mathcal{H}$  [31, Section 5.1].

Two operators  $S$  and  $T$  in  $\mathcal{H}$  are said to be equal, written  $S = T$ , if they have the same domain and  $Sf = Tf$  for all  $f \in \mathcal{D}(S) = \mathcal{D}(T)$ . If  $\mathcal{D}(S) \subset \mathcal{D}(T)$  and  $Sf = Tf$  for all  $f \in \mathcal{D}(S)$ , then we say that  $S$  is a *restriction* of  $T$  and/or  $T$  is an *extension* of  $S$ , and we write  $S \subset T$ . Clearly  $S = T$  if and only if both  $S \subset T$  and  $T \subset S$ . The *sum* of  $S$  and  $T$ , denoted  $S + T$ , is the linear operator in  $\mathcal{H}$  defined by

$$\mathcal{D}(S + T) = \mathcal{D}(S) \cap \mathcal{D}(T) \quad \text{and} \quad (S + T)f = Sf + Tf \quad \text{for } f \in \mathcal{D}(S + T).$$

(The difference  $S - T$  is defined analogously.) The *composition* of  $S$  with  $T$ , denoted  $TS$ , is the operator defined by

$$\mathcal{D}(TS) = \{f \in \mathcal{D}(S) : Sf \in \mathcal{D}(T)\} \quad \text{and} \quad (TS)f = T(Sf) \quad \text{for } f \in \mathcal{D}(TS).$$

Let  $n$  be a nonnegative integer. The  *$n$ :th power* of  $T$  is defined inductively by letting  $T^0 = I$  if  $n = 0$  and  $T^n = TT^{n-1}$  otherwise. We say that  $S$  is an  *$n$ :th root* of  $T$  if  $T = S^n$ .

A linear operator  $S$  is said to be *closable* if it has a closed extension  $T$ . This implies that  $(\mathcal{D}(S), \langle \cdot, \cdot \rangle_S)$  is an inner product subspace of the Hilbert space  $(\mathcal{D}(T), \langle \cdot, \cdot \rangle_T)$ . The closure of the former in the latter is a Hilbert subspace of  $(\mathcal{D}(T), \langle \cdot, \cdot \rangle_T)$ , and thus this closure is the domain of a closed restriction of  $T$ . This restriction is called the *closure* of  $S$ , and is denoted  $\bar{S}$ . There are other equivalent ways to define the closure [31, Section 5.1]; in particular, it can be done in a manner independent of  $T$ . Hence  $\bar{S}$  is uniquely determined by  $S$ , and has the property that  $S \subset \bar{S} \subset T$  for any closed extension  $T$  of  $S$ .

## 2.5 Some important classes of linear operators

Let  $T$  be an operator in a Hilbert space  $\mathcal{H}$ . We say that  $T$  is *symmetric* if

$$\langle Tf, g \rangle = \langle f, Tg \rangle \quad \text{for all } f, g \in \mathcal{D}(T).$$

An equivalent condition is that  $\langle Tf, f \rangle$  is real for all  $f \in \mathcal{D}(T)$  [28, Lemma 3.1]. If  $T$  is everywhere defined and symmetric, then  $T$  is bounded by the Hellinger-Toeplitz theorem [31, Theorem 5.7].

**Lemma 2.1.** *If  $T$  is closable and symmetric, then  $\overline{T}$  is also symmetric.*

*Proof.* We use an equivalent definition of the closure [31, Section 5.1]: For any  $f, g \in \mathcal{D}(\overline{T})$  there exists a sequence  $\{f_n\}$  (resp.  $\{g_n\}$ ) such that  $f_n \rightarrow f$  and  $Tf_n \rightarrow \overline{T}f$  (resp.  $g_n \rightarrow g$  and  $Tg_n \rightarrow \overline{T}g$ ). Hence

$$\langle \overline{T}f, g \rangle = \lim_n \langle Tf_n, g_n \rangle = \lim_n \langle f_n, Tg_n \rangle = \langle f, \overline{T}g \rangle.$$

□

We say that a densely defined symmetric operator  $T$  is *lower semibounded* if there exists  $m \in \mathbb{R}$  such that

$$\langle Tf, f \rangle \geq m \|f\|^2 \quad \text{for all } f \in \mathcal{D}(T).$$

Any such  $m$  is called a *lower bound* of  $T$ , and we write  $T \geq m$ . The least upper bound of all lower bounds of  $T$  is again a lower bound of  $T$ , and is denoted  $\mathbf{m}(T)$ . We say that the lower semibounded operator  $T$  is *nonnegative* if  $\mathbf{m}(T) \geq 0$  and that it is *positive* if  $\mathbf{m}(T) > 0$ . If  $T_1, T_2$  are lower semibounded operators and  $T_1 \subset T_2$ , then  $\mathbf{m}(T_2) \geq \mathbf{m}(T_1)$  as we now show:

$$\mathbf{m}(T_2) = \inf_{\substack{f \in \mathcal{D}(T_2) \\ \|f\|=1}} \langle T_2 f, f \rangle \leq \inf_{\substack{f \in \mathcal{D}(T_1) \\ \|f\|=1}} \langle T_2 f, f \rangle = \inf_{\substack{f \in \mathcal{D}(T_1) \\ \|f\|=1}} \langle T_1 f, f \rangle = \mathbf{m}(T_1).$$

**Lemma 2.2.** *If  $T$  is closable and lower semibounded, then  $\mathbf{m}(\overline{T}) = \mathbf{m}(T)$ .*

*Proof.* On the one hand  $T \subset \overline{T}$  implies  $\mathbf{m}(T) \geq \mathbf{m}(\overline{T})$ . Let  $\epsilon > 0$ . We can find  $f \in \mathcal{D}(\overline{T})$  such that  $\|f\| = 1$  and  $\langle \overline{T}f, f \rangle - \mathbf{m}(\overline{T}) < \epsilon$ . By using an equivalent definition of the closure [31, Section 5.1] we can find  $g \in \mathcal{D}(T)$  such that  $\|g\| = 1$  and  $\langle Tg, g \rangle - \langle \overline{T}f, f \rangle < \epsilon$ . Adding these two inequalities gives  $\langle Tg, g \rangle - \mathbf{m}(\overline{T}) < 2\epsilon$ , and hence  $\mathbf{m}(T) \leq \langle Tg, g \rangle < \mathbf{m}(\overline{T}) + 2\epsilon$ . Since  $\epsilon$  was arbitrary,  $\mathbf{m}(T) \leq \mathbf{m}(\overline{T})$ . □

Let  $T$  be a densely defined operator in  $\mathcal{H}$ . The *adjoint operator* of  $T$ , denoted  $T^*$ , is the linear operator in  $\mathcal{H}$  defined as follows:  $f \in \mathcal{D}(T^*)$  if and only if there exists  $u_f \in \mathcal{H}$  such that  $\langle f, Tg \rangle = \langle u_f, g \rangle$  for all  $g \in \mathcal{D}(T)$ , and in this case  $T^*f = u_f$ . (The element  $u_f$  is uniquely determined by density, so the action of  $T^*$  on  $f$  is well-defined.) One can show that the adjoint operator  $T^*$  is always closed [31, Theorem 5.3]. Furthermore,  $\mathcal{N}(T^*) = \mathcal{R}(T)^\perp$  and  $(T+z)^* = T^* + \bar{z}$  for all  $z \in \mathbb{C} \setminus \{0\}$  [31, Theorems 4.13(b) and 4.20].

We say that a densely defined operator  $T$  is *self-adjoint* if  $T = T^*$ . If  $T$  is an everywhere defined self-adjoint operator, then  $T$  is bounded by the Hellinger-Toeplitz theorem. (Such operators are sometimes called “Hermitian” in analogy with Hermitian matrices, but we will not use this terminology.) We

will use  $\mathcal{B}_{sa}(\mathcal{H})$  to denote the vector space of all everywhere defined self-adjoint operators in  $\mathcal{H}$ , though we warn the reader that this notation is not standard. (It is used in for example [27].)

A densely defined operator  $T$  is symmetric if and only if  $T \subset T^*$ . This implies that all densely defined symmetric operators are closable.

**Proposition 2.3** ([31, Theorem 7.20(a)]). *Let  $A$  be a positive self-adjoint operator. Then  $A$  has a unique positive self-adjoint  $n$ :th root, denoted  $A^{1/n}$ .*

A *partial isometry* on  $\mathcal{H}$  is an everywhere defined operator  $U$  on  $\mathcal{H}$  for which there exists a closed subspace  $M \subset \mathcal{H}$  such that

$$\|Uf\| = \|f\| \quad \text{for all } f \in M, \quad Uf = 0 \quad \text{for all } f \in M^\perp.$$

We call  $M$  (resp.  $\mathcal{R}(U)$ ) the initial (resp. final) domain of  $U$ . (This terminology is not standard, but is used in for example [31].)

**Proposition 2.4** ([31, Theorem 7.20(b)]). *Let  $T$  be a densely defined closed operator in  $\mathcal{H}$ . Then  $T$  can be uniquely represented in the form  $T = U_T|T|$ , where  $|T|$  is a positive self-adjoint operator in  $\mathcal{H}$  and  $U_T$  is a partial isometry with initial domain  $\overline{\mathcal{R}(|T|)}$  and final domain  $\overline{\mathcal{R}(T)}$ .*

The decomposition  $T = U_T|T|$  is called the *polar decomposition* of  $T$ . Note that  $|T|$  has a unique positive self-adjoint square root, denoted  $|T|^{1/2}$ . Note also that  $\mathcal{D}(T) \subset \mathcal{D}(|T|) \subset \mathcal{D}(|T|^{1/2})$ .

An *orthogonal projection* on  $\mathcal{H}$  is an everywhere defined self-adjoint operator  $P$  on  $\mathcal{H}$  such that  $P^2 = P$ . One can show the following [31, Section 4.6]: If  $P$  is an orthogonal projection, then  $P$  acts as the identity on  $\mathcal{R}(P)$  and as the constant map sending everything to zero on  $\mathcal{R}(P)^\perp$ . Conversely, if  $M$  is a closed subspace of  $\mathcal{H}$ , then there exists a unique projection  $P_M$  such that  $M = \mathcal{R}(P_M)$ .

## 2.6 Sesquilinear forms in Hilbert spaces

A *sesquilinear form* (or just “*form*”) in  $\mathcal{H}$  is a map  $\mathfrak{t}[\cdot, \cdot] : \mathcal{D}(\mathfrak{t}) \times \mathcal{D}(\mathfrak{t}) \rightarrow \mathbb{C}$ , where  $\mathcal{D}(\mathfrak{t})$  is a linear subspace of  $\mathcal{H}$  and  $\mathfrak{t}[\cdot, \cdot]$  is linear in its first argument and antilinear in its second.  $\mathcal{D}(\mathfrak{t})$  is called the *domain* of  $\mathfrak{t}$ , and we say that the form  $\mathfrak{t}$  is *everywhere defined* (resp. *densely defined*) if  $\mathcal{D}(\mathfrak{t}) = \mathcal{H}$  (resp.  $\mathcal{D}(\mathfrak{t})$  is dense in  $\mathcal{H}$ ). The *quadratic form* associated to  $\mathfrak{t}$  is the map  $\mathfrak{t}[\cdot] : \mathcal{D}(\mathfrak{t}) \rightarrow \mathbb{C}$  defined by

$$\mathfrak{t}[f] := \mathfrak{t}[f, f] \quad \text{for } f \in \mathcal{D}(\mathfrak{t}).$$

We say that the sesquilinear form  $\mathfrak{t}$  is *symmetric* if

$$\mathfrak{t}[f, g] = \overline{\mathfrak{t}[g, f]} \quad \text{for all } f, g \in \mathcal{D}(\mathfrak{t}).$$

The quadratic form of a symmetric sesquilinear form is real-valued. There is a natural partial order on the set of all symmetric forms: Given two symmetric forms  $\mathfrak{s}$  and  $\mathfrak{t}$ , we write  $\mathfrak{s} \leq \mathfrak{t}$  if  $\mathcal{D}(\mathfrak{s}) \supset \mathcal{D}(\mathfrak{t})$  and  $\mathfrak{s}[f] \leq \mathfrak{t}[f]$  for all  $f \in \mathcal{D}(\mathfrak{t})$ .

(Note that the direction of the inclusion of the domains is opposite to what the symbol  $\leq$  might suggest—this is intentional.)

We say that the symmetric form  $\mathfrak{t}$  is *lower semibounded* if there exists  $m \in \mathbb{R}$  such that

$$\mathfrak{t}[f] \geq m \|f\|^2 \quad \text{for all } f \in \mathcal{D}(\mathfrak{t}).$$

Any such  $m$  is called a *lower bound* of  $\mathfrak{t}$ , and we write  $\mathfrak{t} \geq m$ . The least upper bound of all lower bounds of  $\mathfrak{t}$  is again a lower bound of  $\mathfrak{t}$ , and is denoted  $\mathfrak{m}(\mathfrak{t})$ . We say that the lower semibounded form  $\mathfrak{t}$  is *nonnegative* if  $\mathfrak{m}(\mathfrak{t}) \geq 0$ .

If  $\mathfrak{t}$  is a lower semibounded form with lower bound  $m$ , then its domain  $\mathcal{D}(\mathfrak{t})$  is an inner product space with inner product

$$\langle f, g \rangle_{\mathfrak{t}} := \mathfrak{t}[f, g] + (1 - m)\langle f, g \rangle \quad \text{for } f, g \in \mathcal{D}(\mathfrak{t}).$$

The corresponding induced norm  $\|f\|_{\mathfrak{t}} := \sqrt{\langle f, f \rangle_{\mathfrak{t}}}$  on  $\mathcal{D}(\mathfrak{t})$  is called the *form norm* of  $\mathfrak{t}$ . Replacing  $m$  with any other lower bound gives an equivalent norm [28, Section 10.1]. We say that  $\mathfrak{t}$  is *closed* if  $(\mathcal{D}(\mathfrak{t}), \langle \cdot, \cdot \rangle_{\mathfrak{t}})$  is a Hilbert space with respect to one, hence to all, choices of lower bound  $m$ .

The notions of equality, restriction, extension, and sums of forms are defined as for linear operators. We say that the lower semibounded form  $\mathfrak{s}$  is *closable* if there exists a closed lower semibounded form  $\mathfrak{t}$  such that  $\mathfrak{s} \subset \mathfrak{t}$ , and the closure of  $\mathfrak{s}$ , denoted  $\bar{\mathfrak{s}}$ , is then defined similarly to the closure of a closable operator. One can show that  $\bar{\mathfrak{s}}$  only depends on  $\mathfrak{s}$ , satisfies  $\mathfrak{s} \subset \bar{\mathfrak{s}} \subset \mathfrak{t}$  for any closed extension  $\mathfrak{t}$  of  $\mathfrak{s}$ , and  $\mathfrak{m}(\bar{\mathfrak{s}}) = \mathfrak{m}(\mathfrak{s})$  [28, Section 10.1].

For any  $z \in \mathbb{C}$ , the everywhere defined sesquilinear form  $(f, g) \mapsto z\langle f, g \rangle$  will by a slight abuse of notation be denoted  $z$ . Note that if  $\mathfrak{t}$  is a symmetric form and  $m \in \mathbb{R}$ , then  $\mathfrak{t} \geq m$  in the sense of form orderings if and only if  $\mathfrak{t}[f] \geq m \|f\|^2$  for all  $f \in \mathcal{D}(\mathfrak{t})$ ; that is, if and only if  $\mathfrak{t} \geq m$  in the sense of greatest lower bounds. Thus there is no ambiguity in the notation  $\mathfrak{t} \geq m$ .

## 2.7 The form representation theorem

Let  $A$  be a self-adjoint operator in  $\mathcal{H}$  and let  $A = U_A|A|$  be its polar decomposition. The *sesquilinear form* associated to  $A$  is the sesquilinear form  $\mathfrak{t}_A$  in  $\mathcal{H}$  defined by

$$\mathcal{D}(\mathfrak{t}_A) = \mathcal{D}(|A|^{1/2}) \quad \text{and} \quad \mathfrak{t}_A[f, g] = \langle U_A|A|^{1/2}f, |A|^{1/2}g \rangle \quad \text{for } f, g \in \mathcal{D}(\mathfrak{t}_A).$$

$\mathcal{D}(\mathfrak{t}_A)$  is called the *form domain* of  $A$ . Note that  $\mathfrak{t}_A$  is densely defined since its domain contains  $\mathcal{D}(A)$  and  $A$  is self-adjoint (thus a fortiori densely defined). One can show that  $A$  is lower semibounded if and only if  $\mathfrak{t}_A$  is lower semibounded, in which case  $\mathfrak{t}_A$  is closed and  $\mathfrak{m}(A) = \mathfrak{m}(\mathfrak{t}_A)$  [28, Propositions 10.5(ii) and 10.4(iii)]. The next theorem—the *form representation theorem*—states that we can recover  $A$  from  $\mathfrak{t}_A$  in the case that  $A$  is lower semibounded:

**Theorem 2.5** ([28, Corollary 10.8]). *The map  $A \mapsto \mathfrak{t}_A$  is a bijection of the set of lower semibounded self-adjoint operators onto the set of densely defined lower semibounded closed forms.*

Given a densely defined form  $\mathfrak{t}$ , let  $A_{\mathfrak{t}}$  be the linear operator defined as follows:  $f \in \mathcal{D}(A_{\mathfrak{t}})$  if and only if there exists  $u_f \in \mathcal{D}(\mathfrak{t})$  such that  $\mathfrak{t}[f, g] = \langle u_f, g \rangle$  for all  $g \in \mathcal{D}(\mathfrak{t})$ , and in this case  $A_{\mathfrak{t}} = u_f$ . (The element  $u_f$  is uniquely determined by density, so this action of  $A_{\mathfrak{t}}$  on  $f$  is well-defined.) One can show [28, Theorem 10.7] that when restricted to densely defined lower semibounded closed forms, the map  $\mathfrak{t} \mapsto A_{\mathfrak{t}}$  is the inverse of the map  $A \mapsto \mathfrak{t}_A$  furnished by the form representation theorem.

We define a natural partial order on the set of all lower semibounded self-adjoint operators in  $\mathcal{H}$  by letting  $A \leq B$  if and only if  $\mathfrak{t}_A \leq \mathfrak{t}_B$ . A sufficient (but not necessary) condition for  $A \leq B$  to hold is that  $\mathcal{D}(A) \supset \mathcal{D}(B)$  and  $\langle Af, f \rangle \leq \langle Bf, f \rangle$  for all  $f \in \mathcal{D}(B)$  [28, Section 10.3].

We say that a family  $\{A(\lambda)\}$  of lower semibounded self-adjoint operators indexed by a real parameter  $\lambda$  is *monotonically increasing* if  $A(\lambda_1) \leq A(\lambda_2)$  for all  $\lambda_1 \leq \lambda_2$ , and we say that  $\{A(\lambda)\}$  is *strictly increasing* if it is monotonically increasing and  $A(\lambda_1) \neq A(\lambda_2)$  for all  $\lambda_1 < \lambda_2$ . The notions of monotonically and/or strictly decreasing families are defined similarly.

If  $A$  is self-adjoint and  $m \in \mathbb{R}$ , then  $A \geq m$  in the sense of operator orderings if and only if  $\mathfrak{t}_A \geq m$ , which as we have seen previously is the case if and only if  $\mathfrak{t}_A \geq m$  in the sense of greatest lower bounds. Due to the equality  $\mathfrak{m}(A) = \mathfrak{m}(\mathfrak{t}_A)$ , this is equivalent to  $A \geq m$  in the sense of greatest lower bounds. Thus there is no ambiguity in the notation  $A \geq m$ .

## 2.8 Elementary spectral theory

Let  $T$  be a closed operator in  $\mathcal{H}$  and let  $z \in \mathbb{C}$ . With notation as in Section 2.4, recall that  $T - z$  denotes the operator with domain  $\mathcal{D}(T)$  and action  $f \mapsto Tf - zf$ . The *resolvent set* of  $T$  is the set

$$\rho(T) := \{z \in \mathbb{C} : T - z \text{ is injective and } (T - z)^{-1} \in \mathcal{B}(\mathcal{H})\}.$$

For any  $z \in \rho(A)$ , the operator  $(T - z)^{-1}$  is called the *resolvent of  $T$  at  $z$* . The *spectrum* of  $T$  is the set  $\sigma(T) := \mathbb{C} \setminus \rho(T)$ . The *point spectrum* of  $T$  is a subset of  $\sigma(T)$  and is defined as

$$\sigma_p(T) := \{z \in \mathbb{C} : \mathcal{N}(T - z) \neq \{0\}\}.$$

A point  $z \in \sigma_p(T)$  is called an *eigenvalue* of  $T$ , the (possibly infinite) dimension of  $\mathcal{N}(T - z)$  is called the *multiplicity* of the eigenvalue, and a nonzero  $f \in \mathcal{N}(T - zI)$  is called an *eigenfunction corresponding to the eigenvalue  $z$* . We say that an eigenvalue is *simple* if its multiplicity is 1.

Let  $A$  be self-adjoint. One can show that  $\sigma(A) \subset \mathbb{R}$  [28, Corollary 3.14]. Moreover,  $A$  is lower semibounded if and only if  $\sigma(A)$  is bounded from below, and in this case  $\mathfrak{m}(A) = \min \sigma(A)$  [31, Section 7.4, Corollary 2]. The *discrete spectrum* of  $A$  is a subset of  $\sigma_p(A)$  and is defined as

$$\sigma_d(A) := \{\lambda \in \sigma_p(A) : \lambda \text{ has finite multiplicity and is an isolated point of } \sigma(A)\}.$$

The *essential spectrum* of  $A$  is the set  $\sigma_e(A) := \sigma(A) \setminus \sigma_d(A)$ , and we say that  $A$  has a *purely discrete spectrum* if  $\sigma_e(A) = \emptyset$ .

**Proposition 2.6** ([28, Propositions 5.12, 10.6]). *Let  $A$  be a lower semibounded self-adjoint operator in an infinite dimensional Hilbert space  $\mathcal{H}$ . The following are equivalent:*

- (i)  $A$  has a purely discrete spectrum;
- (ii) the resolvent  $(A - z)^{-1}$  is compact for one, hence for all,  $z \in \rho(A)$ ;
- (iii) the embedding map  $(\mathcal{D}(A), \|\cdot\|_A) \rightarrow (\mathcal{H}, \|\cdot\|)$  is compact;
- (iv) the embedding map  $(\mathcal{D}(\mathfrak{t}_A), \|\cdot\|_{\mathfrak{t}_A}) \rightarrow (\mathcal{H}, \|\cdot\|)$  is compact.

Let  $A$  be as in the above proposition, and suppose that  $A$  has a purely discrete spectrum. Let  $\{\lambda_n\}$  be the increasing sequence of eigenvalues, counted according to their (finite) multiplicity; that is, each eigenvalue appears in the sequence as many times as its multiplicity, and

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$$

The eigenvalue  $\lambda_1$  is called the *principal eigenvalue* of  $A$ . Since  $\mathfrak{m}(A) = \min \sigma(A)$ , we necessarily have  $\lambda_1 = \mathfrak{m}(A)$ .

Let  $F_n$  denote the set of linear subspaces of  $\mathcal{H}$  of codimension  $\leq n$ . (In particular,  $F_0 = \{\mathcal{H}\}$ .) The next theorem is (a special case of) the *Courant-Fischer-Rayleigh min-max principle*:

**Theorem 2.7** ([28, Theorem 12.1]). *Let  $A$  be as in Proposition 2.6, and suppose that  $A$  has a purely discrete spectrum. Then, for all  $n \geq 1$ ,*

$$\lambda_n = \sup_{M \in F_{n-1}} \inf_{\substack{f \in \mathcal{D}(A) \cap M \\ f \neq 0}} \frac{\langle Af, f \rangle}{\|f\|^2} = \sup_{M \in F_{n-1}} \inf_{\substack{f \in \mathcal{D}(\mathfrak{t}_A) \cap M \\ f \neq 0}} \frac{\mathfrak{t}_A[f]}{\|f\|^2}.$$

Taking  $n = 1$  yields the following important special case:

**Corollary 2.8.** *Let  $A$  be as in Theorem 2.7. Then*

$$\lambda_1 = \inf_{\substack{f \in \mathcal{D}(A) \\ f \neq 0}} \frac{\langle Af, f \rangle}{\|f\|^2} = \inf_{\substack{f \in \mathcal{D}(\mathfrak{t}_A) \\ f \neq 0}} \frac{\mathfrak{t}_A[f]}{\|f\|^2}.$$

By using the min-max principle one can show the following result, which explains why the operator ordering is natural.

**Proposition 2.9** ([28, Corollary 12.3]). *Let  $A, B$  be lower semibounded self-adjoint operators in an infinite-dimensional Hilbert space, both with a purely discrete spectrum. If  $A \leq B$ , then  $\lambda_n(A) \leq \lambda_n(B)$  for all  $n$ .*

## 2.9 Defect spaces and defect indices

Let  $T$  be a densely defined symmetric operator in a Hilbert space. Here and in the sequel we use the abbreviation

$$\mathcal{N}_z := \mathcal{N}(T^* - z) \quad \text{for } z \in \mathbb{C}.$$

The *defect space of  $T$  at  $z$*  is the subspace  $\mathcal{R}(T - z)^\perp = \mathcal{N}(T^* - \bar{z}) = \mathcal{N}_{\bar{z}}$ , and the *defect index of  $T$  at  $z$*  is the cardinal number

$$\beta(T, z) := \dim \mathcal{R}(T - z)^\perp = \dim \mathcal{N}(T^* - \bar{z}) = \dim \mathcal{N}_{\bar{z}},$$

where “dim” refers to the Hilbert space dimension, i.e., the cardinality of an orthonormal basis. One can show that the map  $z \mapsto \beta(T, z)$  is constant in the upper and lower half-planes of  $\mathbb{C}$  [31, Theorem 8.1]. The two cardinal numbers  $\beta(T, i)$  and  $\beta(T, -i)$  are called the *defect indices* of  $T$ , and we usually write them as a pair  $(\beta(T, i), \beta(T, -i))$ . Using the so-called von Neumann extension theory, one can show that  $T$  has self-adjoint extensions if and only if the defect indices are equal [31, Theorem 8.6(c)], and if this is the case, then  $\bar{T}$  is self-adjoint if and only if the defect indices are zero [31, Theorem 5.20].

The *regularity domain* of  $T$  is the set

$$\{z \in \mathbb{C} : \text{there exists } c > 0 \text{ such that } \|(T - z)f\| \geq c\|f\| \text{ for all } f \in \mathcal{D}(T)\}.$$

One can show that the regularity domain is open [31, Section 8.1] and the map  $z \mapsto \beta(T, z)$  is constant on each connected component of the regularity domain [31, Theorem 8.1]. If  $T$  is lower semibounded, then one can moreover show that one such component contains the union of the upper- and lower half-planes of  $\mathbb{C}$  together with the portion  $(-\infty, \mathfrak{m}(T))$  of the real line [31, proof of Theorem 8.8]. It follows that the defect indices of  $T$  are equal (so  $T$  has self-adjoint extensions) and that these indices are equal to

$$\beta(T, \lambda) = \dim(\mathcal{N}_\lambda) \quad \text{for each } \lambda < \mathfrak{m}(T).$$

We restate this as a proposition:

**Proposition 2.10.** *Let  $T$  be a densely defined lower semibounded symmetric operator. Then  $T$  has defect indices  $(m, m)$  if and only if  $\dim(\mathcal{N}_\lambda) = m$  for one, hence for all,  $\lambda < \mathfrak{m}(T)$ .*

We shall also need a result from perturbation theory—the subject which studies how the spectrum changes as operators are “perturbed.” This usually means that an operator  $V$  which is in some sense “small” compared to  $T$  is added to the latter to produce a perturbed operator  $T + V$ . For example, under the assumptions of the below proposition and considering  $A$  as a perturbation of  $T_F$ , the difference between the resolvent  $(T_F - z)^{-1}$  and the perturbed resolvent  $(A - z)^{-1}$  is a finite-rank operator with rank at most  $m$  for every  $z \in \rho(T_F) \cap \rho(A)$  [31, Theorem 8.10]. The proposition then follows essentially from this fact.

**Proposition 2.11** ([31, Section 8.4, Corollary 2]). *Let  $T$  be a densely defined lower semibounded symmetric operator with finite defect indices  $(m, m)$ , and let  $A$  be a self-adjoint extension of  $T$ . Then  $\sigma(A) \cap (-\infty, \mathfrak{m}(T))$  consists of only eigenvalues of  $A$  with total multiplicity  $\leq m$ .*

**Corollary 2.12.** *Let  $T$  be a densely defined lower semibounded symmetric operator with finite defect indices. Then all self-adjoint extensions of  $T$  are lower semibounded.*

*Proof.* As we explained in the previous section, a self-adjoint operator is lower semibounded if and only if its spectrum is bounded from below, so the assertion follows immediately from Proposition 2.11.  $\square$

## 2.10 The Friedrichs extension

Let  $T$  be a densely defined lower semibounded operator in a Hilbert space. To  $T$  we associate a densely defined lower semibounded symmetric form  $\mathfrak{s}_T$  by

$$\mathcal{D}(\mathfrak{s}_T) = \mathcal{D}(T) \quad \text{and} \quad \mathfrak{s}_T[f, g] = \langle Tf, g \rangle \quad \text{for} \quad f, g \in \mathcal{D}(\mathfrak{s}_T).$$

One can show that  $\mathfrak{s}_T$  is closable [28, Lemma 10.16]. Let  $\mathfrak{t} = \overline{\mathfrak{s}_T}$ . The *Friedrichs extension* of  $T$  is then defined as the lower semibounded self-adjoint operator  $T_F := A_{\mathfrak{t}}$ , where  $A_{\mathfrak{t}}$  is defined as in Section 2.7.

**Theorem 2.13** ([31, Theorem 10.17]). *Let  $T$  be a densely defined lower semibounded operator and let  $T_F$  be its Friedrichs extension. Then*

- (i)  $T_F$  is a lower semibounded self-adjoint extension of  $T$  with  $\mathfrak{m}(T_F) = \mathfrak{m}(T)$ ;
- (ii) if  $A$  is any lower semibounded self-adjoint extension of  $T$ , then  $A \leq T_F$ ;
- (iii)  $\mathcal{D}(T_F) = \mathcal{D}(T^*) \cap \mathcal{D}(\mathfrak{t})$  and  $T_F = T^* \upharpoonright \mathcal{D}(T_F)$ ;
- (iv)  $(T + \lambda)_F = T_F + \lambda$  for all  $\lambda \in \mathbb{R}$ .

Here  $T^* \upharpoonright \mathcal{D}(T_F)$  denotes the restriction of  $T^*$  to  $\mathcal{D}(T_F)$ .

**Lemma 2.14.** *Let  $\mathfrak{t}$  be a densely defined lower semibounded closed form, and let  $T$  be a densely defined restriction of  $A_{\mathfrak{t}}$ . Then  $T_F = A_{\mathfrak{t}}$  if and only if  $\mathcal{D}(T)$  is dense in  $(\mathcal{D}(\mathfrak{t}), \|\cdot\|_{\mathfrak{t}})$ .*

*Proof.* The form norm of  $\mathfrak{t}$  can be constructed as

$$\|f\|_{\mathfrak{t}}^2 = \mathfrak{t}[f] + (1 - \mathfrak{m}(\mathfrak{t})) \|f\|^2 \quad \text{for} \quad f \in \mathcal{D}(\mathfrak{t}).$$

Since  $\mathfrak{m}(\mathfrak{t}) = \mathfrak{m}(A_{\mathfrak{t}}) \leq \mathfrak{m}(T) = \mathfrak{m}(\mathfrak{s}_T)$ , the form norm of  $\mathfrak{s}_T$  can be constructed as

$$\|f\|_{\mathfrak{s}_T}^2 = \mathfrak{s}_T[f] + (1 - \mathfrak{m}(\mathfrak{t})) \|f\|^2 \quad \text{for} \quad f \in \mathcal{D}(\mathfrak{s}_T).$$

We have  $\mathcal{D}(\mathfrak{s}_T) = \mathcal{D}(T) \subset \mathcal{D}(A_{\mathfrak{t}}) \subset \mathcal{D}(\mathfrak{t})$  and  $\mathfrak{s}_T[f] = \langle Tf, f \rangle = \langle A_{\mathfrak{t}}f, f \rangle = \mathfrak{t}[f]$  for all  $f \in \mathcal{D}(\mathfrak{s}_T)$ , where the last equality follows from the definition of  $A_{\mathfrak{t}}$ .

Hence the two form norms are equal on  $\mathcal{D}(\mathfrak{s}_T)$ , meaning  $(\mathcal{D}(\mathfrak{s}_T), \|\cdot\|_{\mathfrak{s}_T})$  is a normed subspace of  $(\mathcal{D}(\mathfrak{t}), \|\cdot\|_{\mathfrak{t}})$ . The form domain of the Friedrichs extension of  $T$  is by definition the closure of  $\mathcal{D}(\mathfrak{s}_T) = \mathcal{D}(T)$  in  $(\mathcal{D}(\mathfrak{t}), \|\cdot\|_{\mathfrak{t}})$ . We conclude that  $T_F = A_{\mathfrak{t}}$  if and only if this closure is exactly  $\mathcal{D}(\mathfrak{t})$ ; that is, if and only if  $\mathcal{D}(T)$  is dense in  $(\mathcal{D}(\mathfrak{t}), \|\cdot\|_{\mathfrak{t}})$ .  $\square$

### 3 Self-adjoint extension theory

While both [8] and [24] used the extension theory of boundary triplets to construct and parametrize point-interaction Hamiltonians, they did so in rather different ways: The former designed a boundary triplet specifically adapted to the problem at hand, while the latter used what amounts to a generic boundary triplet. The main benefit of the approach used by [24] was that after a physically motivated reparametrization, the authors obtain a connection between the extension parameter and an object called the relative Green's function, and it is this connection that eventually allowed them to derive their Faber-Krahn-type inequality (6). However, [24] only treated the case of a single interaction center. Our aim in this section is therefore to generalize the extension-reparametrization method of [24] until it is applicable to the multi-point case. The main results are Theorem 3.43 and Theorem 3.44, which we consider to be the correct generalizations of their methods to the abstract operator-theoretic setting.

Our source for the Krein-Visik-Birman extension theory is [28], but we would also like to recommend the (at the time of writing) newly published book [5], which treats especially boundary triplets with a great deal of depth.

Henceforth, let  $\mathcal{H}$  be a fixed Hilbert space.

#### 3.1 Parametrizations of self-adjoint extensions

Let  $T$  be a densely defined symmetric operator in  $\mathcal{H}$  and let  $\mathcal{A}$  be the set of all self-adjoint extensions of  $T$ . Assume that  $\mathcal{A}$  is nonempty, which as we explained in Section 2.9 is equivalent to the defect indices of  $T$  being equal. Suppose furthermore that there exist  $A \in \mathcal{A}$  such that  $\rho(A) \cap \mathbb{R}$  is nonempty. Fix any such extension  $A$  and fix  $\lambda \in \rho(A) \cap \mathbb{R}$ . Under these assumptions, we will now describe a way of parametrizing  $\mathcal{A}$  by means of other self-adjoint operators. To this end, recall the abbreviation  $\mathcal{N}_\lambda := \mathcal{N}(T^* - \lambda)$  and let  $\mathcal{S}(\mathcal{N}_\lambda)$  denote the set of all self-adjoint operators in arbitrary closed subspaces of  $\mathcal{N}_\lambda$ ; that is, each  $B \in \mathcal{S}(\mathcal{N}_\lambda)$  corresponds to a pair  $(\mathcal{K}_B, B)$  where  $\mathcal{K}_B$  is a closed subspace of  $\mathcal{N}_\lambda$  and  $B$  is a self-adjoint operator in  $\mathcal{K}_B$ . (This necessitates that both  $\mathcal{D}(B)$  and  $\mathcal{R}(B)$  are subspaces of  $\mathcal{K}_B$ .)

**Theorem 3.1** ([28, Theorem 14.12]). *Let  $T$ ,  $\mathcal{A}$ ,  $A$ , and  $\lambda$  be as above. Then there exists a bijection  $\mathcal{S}(\mathcal{N}_\lambda) \rightarrow \mathcal{A}$ , where the extension  $T_B^\lambda \in \mathcal{A}$  associated to  $B \in \mathcal{S}(\mathcal{N}_\lambda)$  has domain*

$$\mathcal{D}(T_B^\lambda) = \left\{ u = f + (A - \lambda)^{-1}(Bg + h) + g : \begin{array}{l} f \in \mathcal{D}(\overline{T}), g \in \mathcal{D}(B) \\ h \in \mathcal{N}_\lambda \cap \mathcal{D}(B)^\perp \end{array} \right\} \quad (7)$$

and action

$$T_B^\lambda u = \bar{T}f + (I + \lambda(A - \lambda)^{-1})(Bg + h) + \lambda g. \quad (8)$$

Different choices of  $\lambda \in \rho(A) \cap \mathbb{R}$  will in general lead to different parametrizations  $\mathcal{S}(\mathcal{N}_\lambda) \rightarrow \mathcal{A}$  in Theorem 3.1, so it follows that for any pair  $(\lambda, \mu)$  with  $\lambda, \mu \in \rho(A) \cap \mathbb{R}$  there exists a unique reparametrization  $\mathcal{S}(\mathcal{N}_\lambda) \rightarrow \mathcal{S}(\mathcal{N}_\mu)$ , by which we mean a bijection making the following diagram commute:

$$\begin{array}{ccc} \mathcal{S}(\mathcal{N}_\lambda) & \xrightarrow{T^\lambda} & \mathcal{A} \\ \downarrow & \nearrow T^\mu & \\ \mathcal{S}(\mathcal{N}_\mu) & & \end{array} \quad (9)$$

We will have more to say about this later.

Recall that any lower semibounded self-adjoint operator  $A$  is uniquely associated to a densely defined lower semibounded closed form  $\mathfrak{t}_A$ . (See Section 2.7.) As in the next theorem we will sometimes find it convenient to write  $\mathcal{D}[A] := \mathcal{D}(\mathfrak{t}_A)$  for the form domain and  $A[\cdot] := \mathfrak{t}_A[\cdot]$  for the associated quadratic form.

**Theorem 3.2.** *Let  $T$  be a densely defined lower semibounded symmetric operator in  $\mathcal{H}$ . Take  $A = T_F$  and  $\lambda < \mathfrak{m}(T)$  in Theorem 3.1 and let  $B \in \mathcal{S}(\mathcal{N}_\lambda)$ . If  $T_B^\lambda$  is lower semibounded, then*

(i) *the quadratic form of  $T_B^\lambda$  has domain*

$$\mathcal{D}[T_B^\lambda] = \mathcal{D}[T_F] \dot{+} \mathcal{D}[B] \quad (10)$$

and action

$$T_B^\lambda[f + g] = T_F[f] + B[g] + \lambda(\|f + g\|^2 - \|f\|^2) \quad (11)$$

for  $f \in \mathcal{D}[T_B^\lambda]$ ,  $g \in \mathcal{D}[B]$ ;

(ii)  $T_B^\lambda \geq \lambda$  if and only if  $B \geq 0$ .

*Proof.*

(i)  $S := T - \lambda$  is a densely defined positive operator in  $\mathcal{H}$  with Friedrichs extension  $S_F = T_F - \lambda$  by Theorem 2.13(iv). We have

$$\mathfrak{m}(S_F) = \mathfrak{m}(T_F) - \lambda = \mathfrak{m}(T) - \lambda > 0$$

and hence  $0 \in \rho(S_F) \cap \mathbb{R}$ . Moreover,

$$B \in \mathcal{S}(\mathcal{N}_\lambda) = \mathcal{S}(\mathcal{N}(T^* - \lambda)) = \mathcal{S}(\mathcal{N}(S^*)).$$

We may therefore use Theorem 3.1 (with  $T = S$ ,  $A = S_F$ ,  $\lambda = 0$ ) to construct a self-adjoint extension  $S_B^0$  of  $S$ . By comparing the respective expressions (7) and (8) for the two extensions  $T_B^\lambda$  and  $S_B^0$  we see that

$$T_B^\lambda = S_B^0 + \lambda.$$

Now [15, Theorem 2.1 (2.3)] gives

$$\mathcal{D}[T_B^\lambda] = \mathcal{D}[S_B^0] = \mathcal{D}[S_F] \dot{+} \mathcal{D}[B] = \mathcal{D}[T_F] \dot{+} \mathcal{D}[B]$$

which proves (10), while [15, Theorem 2.1 (2.3)] implies

$$(T_B^\lambda - \lambda)[f + g] = S_B^0[f + g] = S_F[f] + B[g] = (T_F - \lambda)[f] + B[g]. \quad (12)$$

Rewriting this expression yields exactly (11).

(ii) The identity (12) tells us that  $T_B^\lambda - \lambda \geq 0$  if and only if

$$(T_F - \lambda)[f] + B[g] \geq 0 \quad \text{for all } f \in \mathcal{D}[T_B^\lambda], g \in \mathcal{D}[B].$$

Recalling the theory of Section 2.7, we have  $\mathfrak{m}(\mathfrak{t}_{T_F - \lambda}) = \mathfrak{m}(T_F - \lambda) > 0$  and therefore  $(T_F - \lambda)[f] > 0$  for all nonzero  $f \in \mathcal{D}[T_B^\lambda]$ . Since in addition  $(T_F - \lambda)[f] = 0$  when  $f = 0$ , we hence conclude from the above inequality that  $B \geq 0$  is both a necessary and sufficient condition for  $T_B^\lambda - \lambda \geq 0$ .  $\square$

The next observation is the author's own.

**Lemma 3.3.** *With the same assumptions as in Theorem 3.2, suppose that  $T$  has finite defect indices  $(m, m)$ . Then each set*

$$\mathcal{A}_n := \{T_B^\lambda : B \in \mathcal{S}(\mathcal{N}_\lambda), \dim(\mathcal{D}(B)) = n\} \quad \text{for } n = 0, 1, \dots, m$$

*is independent of  $\lambda < \mathfrak{m}(T)$ , the sets  $\mathcal{A}_0, \mathcal{A}_1, \dots, \mathcal{A}_m$  are pairwise disjoint, and  $\mathcal{A}_0 \cup \dots \cup \mathcal{A}_m = \mathcal{A}$ .*

*Proof.* Let  $A$  be a self-adjoint extension of  $T$  and let  $B \in \mathcal{S}(\mathcal{N}_\lambda)$  be such that  $A = T_B^\lambda$ . Recall that  $B$  is a self-adjoint operator in some closed subspace  $\mathcal{K}_B$  of  $\mathcal{N}_\lambda$ . Proposition 2.10 implies  $\dim(\mathcal{N}_\lambda) = m$ , so  $\dim(\mathcal{D}(B)) \leq \dim(\mathcal{K}_B) \leq m$ . Moreover, since  $B$  is self-adjoint,  $\mathcal{D}(B)$  is a fortiori a dense subspace of  $\mathcal{K}_B$ , but since both spaces are finite-dimensional we must have  $\mathcal{D}(B) = \mathcal{K}_B$ . The (always valid) chain of inclusions  $\mathcal{D}(B) \subset \mathcal{D}[B] \subset \mathcal{K}_B$  now gives  $\mathcal{D}[B] = \mathcal{D}(B)$ . Corollary 2.12 guarantees that  $A$  is lower semibounded, so the decomposition (10) applies and we have

$$\mathcal{D}[A] = \mathcal{D}[T_F] \dot{+} \mathcal{D}(B).$$

Therefore

$$\mathcal{D}[A]/\mathcal{D}[T_F] \cong \mathcal{D}(B).$$

Since the left-hand side of this isomorphism depends on neither  $\lambda$  nor  $B$ , we see that the integer

$$\dim(\mathcal{D}[A]/\mathcal{D}[T_F]) = \dim(\mathcal{D}(B))$$

only depends on the particular self-adjoint extension  $A$  itself. Thus  $A$  belongs to exactly one of the sets  $\mathcal{A}_0, \dots, \mathcal{A}_m$ , proving both that the sets are independent of  $\lambda$  and cover  $\mathcal{A}$ . The sets are clearly disjoint since each  $A \in \mathcal{A}$  is of the form  $A = T_B^\lambda$  for a unique  $B \in \mathcal{S}(\mathcal{N}_\lambda)$ , and each set is nonempty since we can, for any  $n = 0, 1, \dots, m$ , let  $\mathcal{D}(B)$  be an arbitrary  $n$ -dimensional subspace of  $\mathcal{N}_\lambda$  and  $B$  the identity operator in  $\mathcal{D}(B)$ .  $\square$

We have  $\mathcal{A}_0 = \{T_F\}$  by (10) and (11). As for the other extreme case, recall our notation  $\mathcal{B}_{sa}(\mathcal{N}_\lambda)$  for the vector space of all everywhere defined self-adjoint operators on  $\mathcal{N}_\lambda$ . Since  $\mathcal{D}(B) = m$  if and only if  $B$  is everywhere defined on  $\mathcal{N}_\lambda$ , we have

$$\mathcal{A}_m = \{T_B^\lambda : B \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)\}.$$

The invariance of  $\mathcal{A}_m$  with respect to  $\lambda < \mathbf{m}(T)$  implies that we can restrict our commutative diagram (9) of bijections to the following commutative diagram of bijections:

$$\begin{array}{ccc} \mathcal{B}_{sa}(\mathcal{N}_\lambda) & \xrightarrow{T^\lambda} & \mathcal{A}_m \\ \downarrow & \nearrow T^\mu & \\ \mathcal{B}_{sa}(\mathcal{N}_\mu) & & \end{array} \quad (13)$$

We shall provide a formula for this map  $\mathcal{B}_{sa}(\mathcal{N}_\lambda) \rightarrow \mathcal{B}_{sa}(\mathcal{N}_\mu)$  in Section 3.4.

**Proposition 3.4.** *Let  $T$  be as in Lemma 3.3. If there exist  $f \in \mathcal{N}(T_F - \mathbf{m}(T))$ ,  $\lambda < \mathbf{m}(T)$ ,  $g \in \mathcal{N}_\lambda$  such that  $\langle f, g \rangle \neq 0$ , then  $\mathbf{m}(A) < \mathbf{m}(T)$  for all  $A \in \mathcal{A}_m$ .*

The following proof has been adapted from that of [24, Proposition 4.1(i)].

*Proof.* Let  $B \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)$  be such that  $A = T_B^\lambda$ . We may without loss of generality assume  $\operatorname{Re}\langle f, g \rangle \neq 0$  by replacing  $f$  with  $if$  if necessary. Let

$$\mathcal{L}(t) := T_B^\lambda[f + tg] - \mathbf{m}(T) \|f + tg\|^2 \quad \text{for } t \in \mathbb{R}.$$

Since  $(f, \mathbf{m}(T))$  is an eigenpair of  $T_F$ ,  $T_F[f] = \langle T_F f, f \rangle = \mathbf{m}(T) \|f\|^2$ . Using (11) we arrive after some simplification at

$$\mathcal{L}(t) = t^2 B[g] - (\mathbf{m}(T) - \lambda)(\|f + tg\|^2 - \|f\|^2)$$

in which we note that the first term is  $o(|t|)$  as  $t \rightarrow 0$ . We may also write

$$\|f + tg\|^2 - \|f\|^2 = 2t \operatorname{Re}\langle f, g \rangle + t^2 \|g\|^2$$

in which the second term is  $o(|t|)$  as  $t \rightarrow 0$ . Hence

$$\frac{\mathcal{L}(t)}{t} = -2(\mathbf{m}(T) - \lambda) \operatorname{Re}\langle f, g \rangle + o(1).$$

Since  $\mathcal{L}(0) = 0$ , letting  $t \rightarrow 0$  at both sides yields

$$\mathcal{L}'(0) = -2(\mathbf{m}(T) - \lambda) \operatorname{Re}\langle f, g \rangle \neq 0.$$

Thus by choosing  $t_0$  with small enough absolute value and with correct sign,

$\mathcal{L}(t_0)$  will be negative. Corollary 2.8 then gives

$$\begin{aligned} \mathfrak{m}(A) &= \inf_{h \in \mathcal{D}(T_B^\lambda), h \neq 0} \frac{T_B^\lambda[h]}{\|h\|^2} \\ &\leq \frac{T_B^\lambda[f + t_0g]}{\|f + t_0g\|^2} \\ &= \frac{\mathcal{L}(t_0)}{\|f + t_0g\|^2} + \mathfrak{m}(T) \\ &< \mathfrak{m}(T). \end{aligned}$$

□

### 3.2 Boundary triplets

Let  $T$  be a densely defined symmetric operator in  $\mathcal{H}$ . In the next definition, recall the notion of direct product of Hilbert spaces as defined in Section 2.3.

**Definition 3.5.** A *boundary triplet* for  $T^*$  is a triplet  $(\mathcal{K}, \Gamma_0, \Gamma_1)$  consisting of a Hilbert space  $\mathcal{K}$  and two linear operators  $\Gamma_0, \Gamma_1 : \mathcal{D}(T^*) \rightarrow \mathcal{K}$  such that

- (i) the map  $\mathcal{D}(T^*) \rightarrow \mathcal{K} \oplus \mathcal{K}$  given by  $f \mapsto (\Gamma_0 f, \Gamma_1 f)$  is surjective;
- (ii)  $\langle T^* f, g \rangle - \langle f, T^* g \rangle = \langle \Gamma_1 f, \Gamma_0 g \rangle - \langle \Gamma_0 f, \Gamma_1 g \rangle$  for all  $f, g \in \mathcal{D}(T^*)$ .

The identity in (ii) is sometimes called the *abstract Green identity*.

Recall Section 2.9, in which we defined the defect indices of  $T$  and asserted that  $T$  has self-adjoint extensions if and only if these indices are equal; this is in fact a necessary and sufficient criterion for  $T^*$  to possess a boundary triplet:

**Theorem 3.6** ([28, Proposition 14.5]). *There exists a boundary triplet for  $T^*$  if and only if  $T$  has equal defect indices, in which case the defect indices are equal to  $\dim \mathcal{K}$ , where  $\mathcal{K}$  is the Hilbert space in Definition 3.5.*

In view of the above theorem, let us for the remainder of this section assume that  $T$  has equal defect indices, or equivalently that  $T$  has self-adjoint extensions. Let  $(\mathcal{K}, \Gamma_0, \Gamma_1)$  be a boundary triplet for  $T^*$ . Since  $\mathcal{N}(\Gamma_0), \mathcal{N}(\Gamma_1)$  are subspaces of  $\mathcal{D}(T^*)$ , we can define two distinguished symmetric operators  $T_0, T_1$  in  $\mathcal{H}$  as the restrictions  $T_i := T^* \upharpoonright \mathcal{N}(\Gamma_i)$  for  $i = 0, 1$ . Actually, we have

**Proposition 3.7** ([28, Corollary 14.8]).  *$T_0, T_1$  are self-adjoint extensions of  $T$ .*

Note that this provides the “only if”-part of Theorem 3.6. We now partially prove the “if”-part by constructing a boundary triplet for  $T^*$  in the special case that  $T$  has a self-adjoint extension whose resolvent set contains a real point. For this we need the following proposition, in which  $\dot{+}$  denotes the direct sum of vector spaces and not necessarily an orthogonal sum.

**Proposition 3.8** ([28, Proposition 14.11]). *Let  $A$  be a self-adjoint extension of  $T$ . Then, for each  $z \in \rho(A)$ ,*

$$\mathcal{D}(T^*) = \mathcal{D}(\overline{T}) \dot{+} (A - z)^{-1} \mathcal{N}_{\overline{z}} \dot{+} \mathcal{N}_z, \quad (14)$$

$$\mathcal{D}(A) = \mathcal{D}(\overline{T}) \dot{+} (A - z)^{-1} \mathcal{N}_{\overline{z}}. \quad (15)$$

Let us therefore assume that  $T$  has a self-adjoint extension  $A$  such that  $\rho(A)$  contains a real number  $\lambda$ . We construct a boundary triplet for  $T^*$  as follows: For any  $f \in \mathcal{D}(T^*)$ , the decomposition (14) furnishes three uniquely determined elements  $f_T \in \mathcal{D}(\overline{T})$ ,  $f_0, f_1 \in \mathcal{N}_\lambda$  such that

$$f = f_T + (A - \lambda)^{-1} f_1 + f_0. \quad (16)$$

For  $i = 0, 1$ , define a linear operator  $\Gamma_i^\lambda : \mathcal{D}(T^*) \rightarrow \mathcal{N}_\lambda$  by  $\Gamma_i^\lambda f := f_i$ .

**Proposition 3.9** ([28, Section 14.3]).  *$(\mathcal{N}_\lambda, \Gamma_0^\lambda, \Gamma_1^\lambda)$  is a boundary triplet for  $T^*$ .*

For this particular boundary triplet, the distinguished self-adjoint extension  $T_0$  recovers the self-adjoint extension  $A$  that was used in the construction of the boundary triplet: This is so because (15) and (16) imply

$$\begin{aligned} \mathcal{N}(\Gamma_0^\lambda) &= \{f \in \mathcal{D}(T^*) : \Gamma_0^\lambda f = 0\} \\ &= \{f \in \mathcal{D}(T^*) : f_0 = 0\} \\ &= \{f \in \mathcal{D}(T^*) : f = f_T + (A - \lambda)^{-1} f_1\} \\ &= \mathcal{D}(A). \end{aligned}$$

### 3.3 Gamma fields and Weyl functions

Let  $T$  be a densely defined symmetric operator in  $\mathcal{H}$  with equal defect indices, and let  $(\mathcal{K}, \Gamma_0, \Gamma_1)$  be a boundary triplet for  $T^*$ . As usual, we use  $\|\cdot\|$  to denote the norm induced by the inner product of  $\mathcal{H}$ . Recall also that the restriction of  $T$  to a subspace  $\mathcal{K} \subset \mathcal{D}(T)$  is denoted  $T \upharpoonright \mathcal{K}$ .

**Lemma 3.10** ([28, Lemma 14.13]).

- (i)  $\Gamma_0, \Gamma_1 : (\mathcal{D}(T^*), \|\cdot\|_{T^*}) \rightarrow (\mathcal{K}, \|\cdot\|_{\mathcal{K}})$  are continuous;
- (ii)  $\Gamma_0 \upharpoonright \mathcal{N}_z : (\mathcal{N}_z, \|\cdot\|) \rightarrow (\mathcal{K}, \|\cdot\|_{\mathcal{K}})$  is a continuous bijection for all  $z \in \rho(T_0)$ .

Let  $z \in \rho(T_0)$ . Since  $T^* - z$  is closed, its kernel  $(\mathcal{N}_z, \|\cdot\|)$  is a Banach space, and hence the operator  $(\Gamma_0 \upharpoonright \mathcal{N}_z)^{-1} : (\mathcal{K}, \|\cdot\|_{\mathcal{K}}) \rightarrow (\mathcal{N}_z, \|\cdot\|)$  is bounded by (ii) and the open mapping theorem [14, Theorem 4.6.2].

**Definition 3.11.** The map  $\gamma : \rho(T_0) \rightarrow \mathcal{B}(\mathcal{K}, \mathcal{H})$  defined by  $\gamma(z) := (\Gamma_0 \upharpoonright \mathcal{N}_z)^{-1}$  is called the *gamma field associated to*  $(\mathcal{K}, \Gamma_0, \Gamma_1)$ .

Let  $z \in \rho(T_0)$ . By Lemma 3.10(i) and the boundedness of  $\gamma(z)$  there exist positive constants  $c_1, c_2$  such that

$$\|\Gamma_1 \gamma(z) f\| \leq \|\Gamma_1 \gamma(z) f\|_{T^*} \leq c_1 \|\gamma(z) f\|_{\mathcal{K}} \leq c_1 c_2 \|f\| \quad \text{for all } f \in \mathcal{K}.$$

In other words,  $\Gamma_1 \gamma(z) : (\mathcal{K}, \|\cdot\|_{\mathcal{K}}) \rightarrow (\mathcal{K}, \|\cdot\|_{\mathcal{K}})$  is bounded.

**Definition 3.12.** The map  $M : \rho(T_0) \rightarrow \mathcal{B}(\mathcal{K})$  defined by  $M(z) := \Gamma_1 \gamma(z)$  is called the *Weyl function associated to*  $(\mathcal{K}, \Gamma_0, \Gamma_1)$ .

Note that both the gamma field and Weyl function are operator-valued, and as such are sometimes called *operator fields*.

For our intended purposes, it will be sufficient to only treat those boundary triplets furnished by Proposition 3.9. Thus, for the remainder of this section, let us assume that  $T$  has a self-adjoint extension  $A$  such that  $\rho(A) \cap \mathbb{R}$  is nonempty. Since the induced boundary triplet  $(\mathcal{N}_\lambda, \Gamma_0^\lambda, \Gamma_1^\lambda)$  is dependent on the choice of  $\lambda \in \rho(A) \cap \mathbb{R}$ , the same is true for the associated gamma field and Weyl function, so we will supplement our notation and write  $\gamma_\lambda$  and  $M_\lambda$  for these. Note that these have the form

$$\gamma_\lambda : \rho(A) \rightarrow \mathcal{B}(\mathcal{N}_\lambda, \mathcal{H}) \quad \text{and} \quad M_\lambda : \rho(A) \rightarrow \mathcal{B}(\mathcal{N}_\lambda).$$

Let us write

$$\gamma_\lambda^* : \rho(A) \rightarrow \mathcal{B}(\mathcal{H}, \mathcal{N}_\lambda) \quad \text{and} \quad M_\lambda^* : \rho(A) \rightarrow \mathcal{B}(\mathcal{N}_\lambda)$$

for the pointwise adjoints of the respective operator fields: By this we mean that  $\gamma_\lambda^*(z) := (\gamma_\lambda(z))^*$  and  $M_\lambda^*(z) := (M_\lambda(z))^*$  for all  $z \in \rho(A)$ . Furthermore, although we have  $\gamma_\lambda(z) : \mathcal{N}_\lambda \rightarrow \mathcal{H}$  by definition, Lemma 3.10(ii) obviously allows us to restrict the codomain, in which case we would have  $\gamma_\lambda(z) : \mathcal{N}_\lambda \rightarrow \mathcal{N}_z$ . By a slight abuse of notation we will write  $\gamma_\lambda(z)$  for both of these operators, since it will be clear from the context which is meant. By a similar abuse of notation we will sometimes use  $\gamma_\lambda^*(z)$  to denote both the “full” adjoint  $\gamma_\lambda^*(z) : \mathcal{H} \rightarrow \mathcal{N}_\lambda$  and the restricted adjoint  $\gamma_\lambda^*(z) \upharpoonright \mathcal{N}_z : \mathcal{N}_z \rightarrow \mathcal{N}_\lambda$ .

While we cannot say much in the case of an arbitrary boundary triplet, the gamma field and Weyl functions associated to  $(\mathcal{N}_\lambda, \Gamma_0, \Gamma_1)$  have concrete formulas in terms of resolvents and projections, as the next proposition shows. (With notation as in Section 2.5, recall that  $P_M$  denotes the unique orthogonal projection such that  $M = \mathcal{R}(P)$ , where  $M$  is a closed subspace of  $\mathcal{H}$ .)

**Proposition 3.13** ([28, Example 14.12]). *For any  $z \in \rho(A)$ ,*

- (i)  $\gamma_\lambda(z) = (A - \lambda)(A - z)^{-1} \upharpoonright \mathcal{N}_\lambda$ ;
- (ii)  $M_\lambda(z) = (z - \lambda)P_{\mathcal{N}_\lambda} \gamma_\lambda(z)$ .

By writing  $A - \lambda = (A - z) + (z - \lambda)$  and inserting into (i) we obtain the alternative and often useful formula

$$\gamma_\lambda(z) = I + (z - \lambda)(A - z)^{-1} \upharpoonright \mathcal{N}_\lambda. \quad (17)$$

Here are some important identities satisfied by  $\gamma_\lambda$  and  $M_\lambda$ . We remark that these identities are valid for arbitrary boundary triplets as long as one makes the necessary modifications, but as mentioned earlier we will not need this result in its complete generality. Parts (iii) and (vi) imply that the gamma field and Weyl function are *operator-valued holomorphic functions* on  $\rho(A)$ —we refer to the appendix for a discussion of such functions. (One can even show that the latter is a so-called Nevanlinna function, but we shall not need this fact here.)

**Theorem 3.14** ([28, Propositions 14.14 and 14.15]). *Let  $z, w \in \rho(A)$ . Then*

(i)  $\mathcal{N}(\gamma_\lambda^*(z)) = (\mathcal{N}_z)^\perp$  and  $\gamma_\lambda^*(z) \upharpoonright \mathcal{N}_z$  is a bijection of  $\mathcal{N}_z$  onto  $\mathcal{N}_\lambda$ ;

(ii)  $\gamma_\lambda(z) = (A - w)(A - z)^{-1}\gamma_\lambda(w)$ ;

(iii)  $\gamma_\lambda(z)$  is holomorphic with derivative  $\frac{d}{dz}\gamma_\lambda(z) = (A - z)^{-1}\gamma_\lambda(z)$ ;

(iv)  $M_\lambda^*(z) = M_\lambda(\bar{z})$ ;

(v)  $M_\lambda(w) - M_\lambda(z) = (w - z)\gamma_\lambda^*(\bar{z})\gamma_\lambda(w)$ ;

(vi)  $M_\lambda(z)$  is holomorphic with derivative  $\frac{d}{dz}M_\lambda(z) = \gamma_\lambda^*(\bar{z})\gamma_\lambda(z)$ .

**Corollary 3.15.** *Let  $z \in \rho(A)$  and  $\lambda, \mu \in \rho(A) \cap \mathbb{R}$ . Then*

(i)  $\gamma_\lambda(z) = \gamma_\mu(z)\gamma_\lambda(\mu)$ ;

(ii)  $(\gamma_\lambda(\mu))^{-1} = \gamma_\mu(\lambda)$ ;

(iii)  $(\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu)(\gamma_\mu^*(z) \upharpoonright \mathcal{N}_z) = \gamma_\lambda^*(z) \upharpoonright \mathcal{N}_z$ ;

(iv)  $(\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu)^{-1} = \gamma_\mu^*(\lambda) \upharpoonright \mathcal{N}_\lambda$ .

*Proof.*

(i) Take  $w = \mu$  in Theorem 3.14(ii) and use Proposition 3.13(i) to rewrite the right-hand side.

(ii) Take  $z = \lambda$  in (i) and observe that Proposition 3.13(i) implies  $\gamma_\lambda(\lambda) = I$ .

(iii) Let  $f \in \mathcal{N}_z$  and  $g \in \mathcal{N}_\lambda$ . Then

$$\begin{aligned} \langle (\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu)(\gamma_\mu^*(z) \upharpoonright \mathcal{N}_z)f, g \rangle &= \langle \gamma_\lambda^*(\mu)\gamma_\mu^*(z)f, g \rangle \\ &= \langle f, \gamma_\mu(z)\gamma_\lambda(\mu)g \rangle \\ &= \langle f, \gamma_\lambda(z)g \rangle \\ &= \langle \gamma_\lambda^*(z)f, g \rangle \\ &= \langle (\gamma_\lambda^*(z) \upharpoonright \mathcal{N}_z)f, g \rangle \end{aligned}$$

where we have used (i) in the third equality.

(iv) Taking  $z = \lambda$  in (iii) yields

$$(\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu)(\gamma_\mu^*(\lambda) \upharpoonright \mathcal{N}_\lambda) = \gamma_\lambda^*(\lambda) \upharpoonright \mathcal{N}_\lambda = I^* \upharpoonright \mathcal{N}_\lambda = I.$$

□

**Corollary 3.16.** *Let  $f, g \in \mathcal{N}_\lambda$ . The map  $z \mapsto \langle M_\lambda(z)f, g \rangle$  is analytic on  $\rho(A)$ , and*

$$\frac{d}{dz}\langle M_\lambda(z)f, g \rangle = \langle \gamma_\lambda(z)f, \gamma_\lambda(\bar{z})g \rangle.$$

*Proof.* By Theorem 3.14(vi),

$$\frac{d}{dz}\langle M_\lambda(z)f, g \rangle = \left\langle \frac{d}{dz}M_\lambda(z)f, g \right\rangle = \langle \gamma_\lambda^*(\bar{z})\gamma_\lambda(z)f, g \rangle = \langle \gamma_\lambda(z)f, \gamma_\lambda(\bar{z})g \rangle.$$

□

For the rest of this section we assume that  $A$  is lower semibounded. As discussed in Section 2.8, this implies that  $\mathfrak{m}(A)$  is equal to the minimum of the spectrum of  $A$ , and consequently  $(-\infty, \mathfrak{m}(A)) \subset \rho(A)$ .

**Proposition 3.17.** *Suppose  $A$  is lower semibounded. For all  $s \leq t < \mathfrak{m}(A)$ ,*

- (i)  $\langle \gamma_s(t)h, h \rangle \geq \|h\|^2$  for all  $h \in \mathcal{H}$ ;
- (ii)  $\langle M_\lambda(t)g, g \rangle \geq \langle M_\lambda(s)g, g \rangle + (t-s)\|\gamma_\lambda(s)g\|^2$  for all  $g \in \mathcal{N}_\lambda$ .

*Proof.*

- (i) Our assumptions imply that  $A-t \geq 0$  and  $t \in \rho(A)$ . Let  $h \in \mathcal{H}$  and  $k := (A-t)^{-1}h$ . Then

$$\langle (A-t)^{-1}h, h \rangle = \langle k, (A-t)k \rangle = \langle (A-t)k, k \rangle \geq 0.$$

Since  $h$  was arbitrary,  $(A-t)^{-1} \geq 0$ . Now the assertion follows from (17).

- (ii) Let  $g \in \mathcal{N}_\lambda$  and  $h := \gamma_\lambda(s)g$ . By Theorem 3.14(v) and Corollary 3.15(i),

$$\begin{aligned} \langle (M_\lambda(t) - M_\lambda(s))g, g \rangle &= (t-s)\langle \gamma_\lambda^*(s)\gamma_\lambda(t)g, g \rangle \\ &= (t-s)\langle \gamma_\lambda(t)g, \gamma_\lambda(s)g \rangle \\ &= (t-s)\langle \gamma_s(t)\gamma_\lambda(s)g, \gamma_\lambda(s)g \rangle \\ &= (t-s)\langle \gamma_s(t)h, h \rangle \\ &\geq (t-s)\|h\|^2, \end{aligned}$$

where we have used (i) in the final inequality.

□

**Corollary 3.18.** *Suppose that  $A$  is lower semibounded. Then  $\mu \mapsto M_\lambda(\mu)$  is strictly increasing on  $(-\infty, \mathfrak{m}(A))$ .*

*Proof.* Let  $s < t < \mathfrak{m}(A)$ . Since  $\gamma_\lambda(s)$  is injective, Proposition 3.17(ii) implies that  $\langle M_\lambda(t)g, g \rangle > \langle M_\lambda(s)g, g \rangle$  for all nonzero  $g \in \mathcal{N}_\lambda$  and the assertion follows. □

**Proposition 3.19** ([28, Statement after Corollary 14.23]). *Suppose  $A$  is lower semibounded. Then  $A$  is equal to the Friedrichs extension of  $T$  if and only if*

$$\lim_{\mu \rightarrow -\infty} \langle M_\lambda(\mu)g, g \rangle = -\infty \quad \text{for all } g \in \mathcal{N}_\lambda \setminus \{0\}.$$

### 3.4 The transition map

The reader should keep in mind that the notation and terminology in this and the next three sections have been introduced by the author for the purposes of this thesis and are not standard. The results as they stand have been derived by the author, which is why we do not provide references.

Henceforth, let  $T$  be a densely defined lower semibounded symmetric operator with finite defect indices  $(m, m)$ , let  $A$  be a self-adjoint extension of  $T$ , and let  $\lambda, \mu \in \rho(A) \cap \mathbb{R}$ . Recall that we write  $\mathcal{B}_{sa}(\mathcal{K})$  for the vector space of everywhere defined (and necessarily bounded) self-adjoint operators in a Hilbert space  $\mathcal{K}$ . Our goal in this section is to describe the unique bijection  $\mathcal{B}_{sa}(\mathcal{N}_\lambda) \rightarrow \mathcal{B}_{sa}(\mathcal{N}_\mu)$  making the diagram (13) commute.

By the theory in the previous section, we have for any  $B \in \mathcal{B}_{sa}(\mathcal{N}_\mu)$  a not necessarily commutative diagram as below, where “ $\sim$ ” indicates a bijection.

$$\begin{array}{ccccccc} \mathcal{N}_\lambda & \xrightarrow[\sim]{\gamma_\lambda(\mu)} & \mathcal{N}_\mu & \xrightarrow{B} & \mathcal{N}_\mu & \xrightarrow[\sim]{\gamma_\lambda^*(\mu)} & \mathcal{N}_\lambda \\ & \searrow & & & & \nearrow & \\ & & & & M_\lambda(\mu) & & \end{array}$$

Theorem 3.14(iv) implies that  $M_\lambda(\mu) \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)$ , so it follows from the above diagram that our choice of  $B$  induces a new everywhere defined self-adjoint operator  $C \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)$  by

$$C := \gamma_\lambda^*(\mu)B\gamma_\lambda(\mu) + M_\lambda(\mu).$$

In this way we obtain a map  $\Gamma(\mu, \lambda) : \mathcal{B}_{sa}(\mathcal{N}_\mu) \rightarrow \mathcal{B}_{sa}(\mathcal{N}_\lambda)$  by

$$\Gamma(\mu, \lambda)B := \gamma_\lambda^*(\mu)B\gamma_\lambda(\mu) + M_\lambda(\mu) \quad \text{for } B \in \mathcal{B}_{sa}(\mathcal{N}_\mu). \quad (18)$$

Recall now the set  $\mathcal{A}_m$  of self-adjoint extensions of  $T$  defined in Lemma 3.3 and note that  $\mathcal{A}_m$  acts as a sort of “manifold of self-adjoint extensions”: For each  $\lambda < \mathfrak{m}(T)$ , Theorem 3.1 furnishes a map  $T^\lambda : \mathcal{B}_{sa}(\mathcal{N}_\lambda) \xrightarrow{\sim} \mathcal{A}_m$  acting as a sort of global coordinate chart, in the sense that  $\mathcal{A}_m$  takes the role of the manifold,  $\mathcal{B}_{sa}(\mathcal{N}_\mu)$  takes the role of the open Euclidean subset,  $B \in \mathcal{B}_{sa}(\mathcal{N}_\mu)$  takes the role of the local coordinate, and  $T_B^\lambda \in \mathcal{A}_m$  takes the role of a point on the manifold. Formally speaking, changing  $\lambda$  to  $\mu$  or vice versa should then, as in manifold theory, induce a *transition map*  $\mathcal{B}_{sa}(\mathcal{N}_\mu) \xrightarrow{\sim} \mathcal{B}_{sa}(\mathcal{N}_\lambda)$  which describes how to pass between the two coordinate systems. The author, based on this, has chosen the following terminology:

**Definition 3.20.**  $\Gamma(\mu, \lambda)$  is called the *transition map* from  $\mu$  to  $\lambda$ .

Our next proposition shows that  $\Gamma(\mu, \lambda)$  has some of the basic properties we would expect from such a map.

**Proposition 3.21.** *Let  $\lambda, \mu, \eta \in \rho(A) \cap \mathbb{R}$ . Then*

- (i)  $\Gamma(\lambda, \lambda)$  is the identity map on  $\mathcal{B}_{sa}(\mathcal{N}_\lambda)$ ;

- (ii)  $\Gamma(\mu, \lambda)M_\mu(\eta) = M_\lambda(\eta)$ ;
- (iii)  $\Gamma(\mu, \lambda)\Gamma(\eta, \mu) = \Gamma(\eta, \lambda)$ ;
- (iv)  $\Gamma(\mu, \lambda)$  is a bijection with inverse  $\Gamma(\mu, \lambda)^{-1} = \Gamma(\lambda, \mu)$ .

*Proof.*

- (i) Proposition 3.13 implies  $\gamma_\lambda(\lambda) = \text{id}_{\mathcal{N}_\lambda}$  and  $M_\lambda(\lambda) = 0$ . Then  $\gamma_\lambda^*(\lambda) = P_{\mathcal{N}_\lambda}$ , and hence  $\gamma_\lambda^*(\lambda) \upharpoonright \mathcal{N}_\lambda = \text{id}_{\mathcal{N}_\lambda}$ . Plugging these into (18) gives that  $\Gamma(\lambda, \lambda)B = B$  for all  $B \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)$ .
- (ii) Theorem 3.14(v) gives

$$M_\mu(\eta) = M_\mu(\eta) - M_\mu(\mu) = (\eta - \mu)\gamma_\mu^*(\mu)\gamma_\mu(\eta).$$

Proposition 3.13(i), Theorem 3.14(v), and (17) then together yields

$$\begin{aligned} \gamma_\lambda^*(\mu)M_\mu(\eta)\gamma_\lambda(\mu) &= (\eta - \mu)\gamma_\lambda^*(\mu)\gamma_\mu^*(\mu)\gamma_\mu(\eta)\gamma_\lambda(\mu) \\ &= (\eta - \mu)(\gamma_\mu(\mu)\gamma_\lambda(\mu))^*(\gamma_\mu(\eta)\gamma_\lambda(\mu)) \\ &= (\eta - \mu)\gamma_\lambda^*(\mu)\gamma_\lambda(\eta) \\ &= M_\lambda(\eta) - M_\lambda(\mu). \end{aligned}$$

Adding  $M_\lambda(\mu)$  to both sides yields exactly  $\Gamma(\mu, \lambda)M_\mu(\eta) = M_\lambda(\eta)$ .

- (iii) Let  $B \in \mathcal{B}_{sa}(\mathcal{N}_\eta)$ . Then, by (ii) and (18),

$$\begin{aligned} \Gamma(\mu, \lambda)\Gamma(\eta, \mu)B &= \Gamma(\mu, \lambda)(\gamma_\mu^*(\eta)B\gamma_\mu(\eta) + \gamma_\mu(\eta)) \\ &= \gamma_\lambda^*(\mu)\gamma_\mu^*(\eta)B\gamma_\mu(\eta)\gamma_\lambda(\mu) + \gamma_\lambda^*(\mu)M_\mu(\eta)\gamma_\lambda(\mu) + M_\lambda(\mu) \\ &= (\gamma_\mu(\eta)\gamma_\lambda(\mu))^*B(\gamma_\mu(\eta)\gamma_\lambda(\mu)) + \Gamma(\mu, \lambda)M_\mu(\eta) \\ &= \gamma_\lambda^*(\eta)B\gamma_\lambda(\eta) + M_\lambda(\eta) \\ &= \Gamma(\eta, \lambda)B. \end{aligned}$$

- (iv) This is an immediate consequence of part (i) and (iii). □

**Lemma 3.22.** *Let  $B \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)$  and suppose that  $\Gamma(\lambda, \mu)B$  is invertible. Then  $B - M_\lambda(\mu)$  is invertible and*

$$(\Gamma(\lambda, \mu)B)^{-1} = \gamma_\lambda(\mu)(B - M_\lambda(\mu))^{-1}(\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu).$$

*Proof.* Let  $C := \Gamma(\lambda, \mu)B$ . Then  $B = \Gamma(\mu, \lambda)C$ , so we have

$$B = \gamma_\lambda^*(\mu)C\gamma_\lambda(\mu) + M_\lambda(\mu)$$

by definition of the transfer map. Thus

$$B - M_\lambda(\mu) = \gamma_\lambda^*(\mu)C\gamma_\lambda(\mu)$$

in which we see that the right-hand side, and therefore also the left-hand side, is invertible. Inverting both sides yields

$$(B - M_\lambda(\mu))^{-1} = (\gamma_\lambda(\mu))^{-1} C^{-1} (\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu)^{-1}$$

and consequently

$$\gamma_\lambda(\mu)(B - M_\lambda(\mu))^{-1}(\gamma_\lambda^*(\mu) \upharpoonright \mathcal{N}_\mu) = C^{-1}.$$

□

We can now prove (under the assumption that  $T$  has finite defect indices) that the transfer map is the unique map making the following diagram commute:

$$\begin{array}{ccc} \mathcal{B}_{sa}(\mathcal{N}_\lambda) & \xrightarrow{T^\lambda} & \mathcal{A}_m \\ \Gamma(\lambda, \mu) \downarrow & \nearrow T^\mu & \\ \mathcal{B}_{sa}(\mathcal{N}_\mu) & & \end{array} \quad (19)$$

**Theorem 3.23.**  $T_B^\lambda = T_{\Gamma(\lambda, \mu)B}^\mu$  for all  $B \in \mathcal{B}_{sa}(\mathcal{N}_\lambda)$ .

*Proof.* Corollary 2.12 implies that  $T_B^\lambda$  is lower semibounded, so we may choose  $\eta < \min\{\mathfrak{m}(T_B^\lambda), \mathfrak{m}(A)\}$ . The Krein-Naimark resolvent formula [28, Theorem 14.18] when applied to the extension  $T_B^\lambda$  states that  $B - M_\lambda(\eta)$  is invertible and

$$(T_B^\lambda - \eta)^{-1} - (A - \eta)^{-1} = \gamma_\lambda(\eta)(B - M_\lambda(\eta))^{-1} \gamma_\lambda^*(\eta).$$

Theorem 3.14(i) implies that we can write  $\gamma_\lambda^*(\eta) = (\gamma_\lambda^*(\eta) \upharpoonright \mathcal{N}_\eta) P_{\mathcal{N}_\eta}$  where  $P_{\mathcal{N}_\eta}$  denotes the orthogonal projection onto  $\mathcal{N}_\eta$ , and we may hence use Lemma 3.22 to substitute in the above formula and obtain

$$(T_B^\lambda - \eta)^{-1} - (A - \eta)^{-1} = (\Gamma(\lambda, \eta)B)^{-1} P_{\mathcal{N}_\eta}.$$

Lemma 3.3 next implies that there exists a unique  $C \in \mathcal{B}_{sa}(\mathcal{N}_\mu)$  such that  $T_B^\lambda = T_C^\mu$ . Arguing as above we find

$$(T_C^\mu - \eta)^{-1} - (A - \eta)^{-1} = (\Gamma(\mu, \eta)C)^{-1} P_{\mathcal{N}_\eta}.$$

Since the left-hand sides of the respective resolvent formulas are equal, we obtain

$$(\Gamma(\lambda, \eta)B)^{-1} P_{\mathcal{N}_\eta} = (\Gamma(\mu, \eta)C)^{-1} P_{\mathcal{N}_\eta}$$

which implies

$$\Gamma(\lambda, \eta)B = \Gamma(\mu, \eta)C$$

and, using Proposition 3.21,

$$C = \Gamma(\mu, \eta)^{-1} \Gamma(\lambda, \eta)B = \Gamma(\eta, \mu) \Gamma(\lambda, \eta)B = \Gamma(\lambda, \mu)B.$$

□

### 3.5 Gamma families and Weyl matrices

Let  $T$  and  $A$  be as in the previous section and let  $(m, m)$  be the (finite) defect indices of  $T$ . Proposition 2.10 implies that  $\dim(\mathcal{N}_\mu) = m$  for all  $\mu \in \rho(A) \cap \mathbb{R}$ . In fact, it suffices to know this for one particular  $\mu$ , since  $\gamma_\mu(\lambda)$  is a vector space isomorphism of  $\mathcal{N}_\mu$  onto  $\mathcal{N}_\lambda$  and therefore  $\dim(\mathcal{N}_\lambda) = \dim(\mathcal{N}_\mu) = m$  for all  $\lambda \in \rho(A) \cap \mathbb{R}$ . More precisely, any ordered basis  $\mathbb{E}_\mu = (e_\mu^1, \dots, e_\mu^m)$  of  $\mathcal{N}_\mu$  induces an ordered basis  $\mathbb{E}_\lambda = (e_\lambda^1, \dots, e_\lambda^m)$  of  $\mathcal{N}_\lambda$  by letting  $e_\lambda^i := \gamma_\mu(\lambda)e_\mu^i$  for each  $i = 1, \dots, m$ . Let us abbreviate this relationship as

$$\mathbb{E}_\lambda = \gamma_\mu(\lambda)\mathbb{E}_\mu. \quad (20)$$

By Corollary 3.15(i), we then conversely have  $\gamma_\lambda(\mu)\mathbb{E}_\lambda = \mathbb{E}_\mu$ , so just as  $\mathbb{E}_\mu$  is said to induce  $\mathbb{E}_\lambda$  we may also say that  $\mathbb{E}_\lambda$  induces  $\mathbb{E}_\mu$ , or more generally that they induce each other. This motivates our next pair of definitions:

**Definition 3.24.** Let  $\mathbb{E}_\mu$  and  $\mathbb{E}_\lambda$  be ordered bases of  $\mathcal{N}_\mu$  and  $\mathcal{N}_\lambda$ , respectively. We say that  $\mathbb{E}_\mu$  and  $\mathbb{E}_\lambda$  are *gamma compatible* if (20) holds.

**Definition 3.25.** Let  $\mathcal{J}$  be a nonempty subset of  $\rho(A) \cap \mathbb{R}$ . A *gamma family* for  $(T, A)$  on  $\mathcal{J}$  is a family  $\mathbb{E} = \{\mathbb{E}_\mu : \mu \in \mathcal{J}\}$  of gamma compatible bases, where  $\mathbb{E}_\mu$  is a basis of  $\mathcal{N}_\mu$  for each  $\mu \in \mathcal{J}$ .

Note that the concept of a gamma family only makes sense with respect to a pair  $(T, A)$  and not the operator  $T$  by itself. This is because changing the self-adjoint extension  $A$  will in general change the gamma field and thus the criterion of gamma compatibility. Note also that to specify a gamma family on  $\mathcal{J}$ , it suffices to specify  $\mathbb{E}_\mu$  for a single  $\mu \in \mathcal{J}$ ; all the other bases in the family are then uniquely specified by gamma compatibility. Finally, note that we may always uniquely extend a gamma family defined on a subset of  $\rho(A) \cap \mathbb{R}$  to a “full” gamma family on  $\rho(A) \cap \mathbb{R}$ . Our reason for allowing a smaller set  $\mathcal{J}$  in the definition is this: In our intended application of these concepts (Section 4.4),  $T$  will be a lower semibounded differential operator with a purely discrete spectrum,  $A = T_F$  will be the Friedrichs extension,  $(A - \lambda)^{-1}$  will be an integral operator for all  $\lambda \in \mathcal{J} := (-\infty, \mathfrak{m}(T))$ , and we will construct a designated gamma family for  $(T, T_F)$  on  $\mathcal{J}$  using the kernels of these integral operators.

Let  $\mathbb{E}$  be a gamma family for  $(T, A)$  on  $\mathcal{J}$ , and let  $\mu \in \mathcal{J}$ . For each vector  $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_m)^T \in \mathbb{C}^m$ , define a corresponding element  $\mathbf{u}_\mu \in \mathcal{N}_\mu$  by

$$\mathbf{u}_\mu := \sum_i \mathbf{u}_i e_\mu^i.$$

This yields a vector space isomorphism  $U_\mu : \mathbb{C}^m \rightarrow \mathcal{N}_\mu$  by letting  $U_\mu \mathbf{u} := \mathbf{u}_\mu$ . The defining property of  $\mathbb{E}$ , namely the requirement that the bases in  $\mathbb{E}$  are gamma compatible, is then equivalent to the commutation relation

$$U_\lambda = \gamma_\mu(\lambda)U_\mu \quad \text{for all } \lambda, \mu \in \mathcal{J}. \quad (21)$$

Let  $\mathcal{M}_{sa}(m)$  denote the vector space of complex Hermitian  $m \times m$  matrices. For each everywhere defined self-adjoint operator  $B \in \mathcal{B}_{sa}(\mathcal{N}_\mu)$ , define a corresponding matrix  $\mathbf{B} = (\mathbf{B}_{ij})_{ij} \in \mathcal{M}_{sa}(m)$  by letting

$$\mathbf{B}_{ij} := \langle B e_\mu^j, e_\mu^i \rangle \quad \text{for all } i, j = 1, \dots, m.$$

This is equivalent to the requirement

$$\langle B \mathbf{u}_\mu, \mathbf{v}_\mu \rangle = \mathbf{v}^H \mathbf{B} \mathbf{u} \quad \text{for all } \mathbf{u}, \mathbf{v} \in \mathbb{C}^m.$$

**Definition 3.26.**  $\mathbf{B}$  is called the  $\mathbb{E}$ -matrix of  $B$ .

Conversely, for each matrix  $\mathbf{B} \in \mathcal{M}_{sa}(m)$ , we may define a corresponding operator  $\mathbf{B}_\mu \in \mathcal{N}_\mu$  as the unique everywhere defined self-adjoint operator whose associated sesquilinear form is given by

$$\mathbf{B}_\mu[\mathbf{u}_\mu, \mathbf{v}_\mu] = \langle \mathbf{B}_\mu \mathbf{u}_\mu, \mathbf{v}_\mu \rangle = \mathbf{v}^H \mathbf{B} \mathbf{u} \quad \text{for all } \mathbf{u}, \mathbf{v} \in \mathbb{C}^m. \quad (22)$$

If  $\mathbf{B}$  is the  $\mathbb{E}$ -matrix of  $B$ , then clearly  $\mathbf{B}_\mu = B$ . In this way we obtain another vector space isomorphism

$$\begin{aligned} \mathcal{M}_{sa}(m) &\xrightarrow{\sim} \mathcal{B}_{sa}(\mathcal{N}_\mu) \\ \mathbf{B} &\longmapsto \mathbf{B}_\mu. \end{aligned} \quad (23)$$

**Proposition 3.27.** Let  $\lambda, \mu \in \mathcal{J}$ . Then

$$\mathbf{B}_\lambda = \gamma_\lambda^*(\mu) \mathbf{B}_\mu \gamma_\lambda(\mu) \quad \text{for all } \mathbf{B} \in \mathcal{M}_{sa}(m).$$

*Proof.* Let  $\mathbf{u}, \mathbf{v} \in \mathbb{C}^m$ . Then, by (21) and (22),

$$\begin{aligned} \langle \gamma_\lambda^*(\mu) \mathbf{B}_\mu \gamma_\lambda(\mu) \mathbf{u}_\lambda, \mathbf{v}_\lambda \rangle &= \langle \mathbf{B}_\mu \gamma_\lambda(\mu) \mathbf{u}_\lambda, \gamma_\lambda(\mu) \mathbf{v}_\lambda \rangle = \langle \mathbf{B}_\mu \mathbf{u}_\mu, \mathbf{v}_\mu \rangle \\ &= \mathbf{v}^H \mathbf{B} \mathbf{u} = \langle \mathbf{B}_\lambda \mathbf{u}_\lambda, \mathbf{v}_\lambda \rangle. \end{aligned}$$

Since  $\{\mathbf{v}_\lambda : \mathbf{v} \in \mathbb{C}^m\} = \mathcal{N}_\lambda$  the assertion follows.  $\square$

The simplest nontrivial  $\mathbb{E}$ -matrix one is likely to think of is the  $\mathbb{E}$ -matrix of the identity operator. It will play an important role in the sequel, so we give this matrix its own notation:

**Definition 3.28.** The  $\mathbb{E}$ -matrix of the identity operator in  $\mathcal{N}_\mu$  is denoted  $\mathbf{E}(\mu)$ .

By definition,  $\mathbf{E}(\mu)$  is the unique  $m \times m$  matrix such that

$$\langle \mathbf{u}_\mu, \mathbf{v}_\mu \rangle = \mathbf{v}^H \mathbf{E}(\mu) \mathbf{u} \quad \text{for all } \mathbf{u}, \mathbf{v} \in \mathbb{C}^m. \quad (24)$$

That is,  $\mathbf{E}(\mu) = (\langle e_\mu^j, e_\mu^i \rangle)_{ij}$ , where  $\langle \cdot, \cdot \rangle$  as usual denotes the inner product of the ambient Hilbert space  $\mathcal{H}$ . Since the restriction of the inner product to  $\mathcal{N}_\mu$  is again an inner product, we see from the above identity that  $\mathbf{E}(\mu)$  is a positive definite Hermitian matrix. (Of course, the Hermitian part is already guaranteed

due to  $\mathbf{E}(\mu)$  being an  $\mathbb{E}$ -matrix.) In particular,  $\mathbb{E}_\mu$  is an orthonormal basis if and only if  $\mathbf{E}(\mu)$  is the identity matrix.

The eigenspaces and operator ordering of operators in  $\mathcal{B}_{sa}(\mathcal{N}_\mu)$  can be expressed in terms of the eigenspaces and operator ordering of their  $\mathbb{E}$ -matrices, as the next lemma shows.

**Lemma 3.29.** *Let  $\mathbf{B}, \mathbf{B}_1, \mathbf{B}_2 \in \mathcal{M}_{sa}(m)$ . Then*

- (i)  $\mathcal{N}(\mathbf{B}_\mu - z) = U_\mu \mathcal{N}(\mathbf{B} - z\mathbf{E}(\mu))$  for all  $z \in \mathbb{C}$ ;
- (ii)  $(\mathbf{B}_1)_\mu \leq (\mathbf{B}_2)_\mu$  if and only if  $\mathbf{B}_1 \leq \mathbf{B}_2$ .

*Proof.*

- (i) Using (22), we have

$$\begin{aligned} \mathcal{N}(\mathbf{B}_\mu) &= \{\mathbf{u}_\mu : \mathbf{B}_\mu \mathbf{u}_\mu = 0\} \\ &= \{U_\mu \mathbf{u} : \langle \mathbf{B}_\mu \mathbf{u}_\mu, \mathbf{v}_\mu \rangle = 0 \text{ for all } \mathbf{v} \in \mathbb{C}^m\} \\ &= U_\mu \{\mathbf{u} : \mathbf{v}^H \mathbf{B} \mathbf{u} = 0 \text{ for all } \mathbf{v} \in \mathbb{C}^m\} \\ &= U_\mu \{\mathbf{u} : \mathbf{B} \mathbf{u} = 0\} \\ &= U_\mu \mathcal{N}(\mathbf{B}). \end{aligned}$$

This proves the case  $z = 0$ . Since  $\mathbf{B} \mapsto \mathbf{B}_\mu$  is linear,  $(\mathbf{B} - z\mathbf{E}(\mu))_\mu = \mathbf{B}_\mu - z\mathbf{E}(\mu)_\mu = \mathbf{B}_\mu - z$  for all  $z \in \mathbb{C}$ , and hence

$$\mathcal{N}(\mathbf{B}_\mu - z) = \mathcal{N}((\mathbf{B} - z\mathbf{E}(\mu))_\mu) = U_\mu \mathcal{N}(\mathbf{B} - z\mathbf{E}(\mu)).$$

- (ii) (22) implies that  $(\mathbf{B}_i)_\mu[\mathbf{u}_\mu] = \mathbf{B}_i[\mathbf{u}]$  for all  $\mathbf{u} \in \mathbb{C}^m$  and  $i \in \{1, 2\}$  in the sense of quadratic forms. Hence  $(\mathbf{B}_1)_\mu[\mathbf{u}_\mu] \leq (\mathbf{B}_2)_\mu[\mathbf{u}_\mu]$  for all  $\mathbf{u} \in \mathbb{C}^m$  if and only if  $\mathbf{B}_1[\mathbf{u}] \leq \mathbf{B}_2[\mathbf{u}]$  for all  $\mathbf{u} \in \mathbb{C}^m$ . This is equivalent to the assertion. □

Let  $\lambda \in \mathcal{J}$ . Recall from Section 3.3 that  $T^*$  has a designated boundary triplet  $(\mathcal{N}_\lambda, \Gamma_0^\lambda, \Gamma_1^\lambda)$ , and let as usual  $M_\lambda : \rho(A) \rightarrow \mathcal{B}(\mathcal{N}_\lambda)$  denote the Weyl function associated to  $(\mathcal{N}_\lambda, \Gamma_0^\lambda, \Gamma_1^\lambda)$ . For our purposes, the single most important  $\mathbb{E}$ -matrix will be the  $\mathbb{E}$ -matrix of  $M_\lambda(\mu)$  and deserves its own name:

**Definition 3.30.** The  $\mathbb{E}$ -matrix of  $M_\lambda(\mu)$  is called the *Weyl matrix* and is denoted  $\mathbf{M}(\mu, \lambda)$ .

Be mindful of the many implicit dependencies in this definition:  $\mathbf{M}(\mu, \lambda)$  depends on  $\lambda, \mu$  and the Weyl function, while the Weyl function depends on the boundary triplet, and the boundary triplet finally depends on the particular self-adjoint extension  $A$  of  $T$ . So as to not clutter the terminology, we suppress most of these and just call  $\mathbf{M}(\mu, \lambda)$  the Weyl matrix. Now would also be a good time to remind the reader that the material in this and the next section

is original to this thesis, so it is unlikely that the name ‘‘Weyl matrix’’ would have the same meaning anywhere else.

By definition,  $\mathbf{M}(\mu, \lambda)$  is the unique  $m \times m$  matrix such that,

$$\mathbf{M}(\mu, \lambda) = (\langle M_\lambda(\mu) e_\lambda^j, e_\lambda^i \rangle)_{ij} \quad \text{for all } i, j = 1, \dots, m.$$

The sesquilinear form of  $\mathbf{M}(\mu, \lambda)$  has a nice and symmetric appearance:

**Lemma 3.31.**  $\mathbf{v}^H \mathbf{M}(\mu, \lambda) \mathbf{u} = (\mu - \lambda) \langle \mathbf{u}_\mu, \mathbf{v}_\lambda \rangle$  for all  $\mathbf{u}, \mathbf{v} \in \mathbb{C}^m$ .

*Proof.* By the definition of the Weyl matrix, (22), and Proposition 3.13(ii),

$$\begin{aligned} \mathbf{v}^H \mathbf{M}(\mu, \lambda) \mathbf{u} &= \langle (\mu - \lambda) P_{\mathcal{N}_\lambda} \gamma_\lambda(\mu) \mathbf{u}_\lambda, \mathbf{v}_\lambda \rangle = (\mu - \lambda) \langle \mathbf{u}_\mu, P_{\mathcal{N}_\lambda} \mathbf{v}_\lambda \rangle \\ &= (\mu - \lambda) \langle \mathbf{u}_\mu, \mathbf{v}_\lambda \rangle. \end{aligned}$$

□

We can now characterize the transfer map in terms of the Weyl matrix, which was in fact the author’s main motivation for introducing gamma families and  $\mathbb{E}$ -matrices in the first place.

**Theorem 3.32.**  $\Gamma(\mu, \lambda) \mathbf{B}_\mu = (\mathbf{B} + \mathbf{M}(\mu, \lambda))_\lambda$  for all  $\mathbf{B} \in \mathcal{M}_{sa}(m)$ .

*Proof.* By (18), Proposition 3.27, the linearity of  $\mathbf{B} \mapsto \mathbf{B}_\lambda$ , and the definition of the Weyl matrix, we have

$$\Gamma(\mu, \lambda) \mathbf{B}_\mu = \gamma_\lambda^*(\mu) \mathbf{B}_\mu \gamma_\lambda(\mu) + M_\lambda(\mu) = \mathbf{B}_\lambda + (\mathbf{M}(\mu, \lambda))_\lambda = (\mathbf{B} + \mathbf{M}(\mu, \lambda))_\lambda.$$

□

The theorem can be viewed as asserting the commutativity of the diagram

$$\begin{array}{ccc} \mathcal{M}_{sa}(m) & \xrightarrow{\sim} & \mathcal{B}_{sa}(\mathcal{N}_\mu) \\ \mathbf{B} \mapsto \mathbf{B} + \mathbf{M}(\mu, \lambda) \downarrow & & \downarrow \Gamma(\mu, \lambda) \\ \mathcal{M}_{sa}(m) & \xrightarrow{\sim} & \mathcal{B}_{sa}(\mathcal{N}_\lambda) \end{array} \quad (25)$$

where the top and bottom bijections are the isomorphisms in (23). We may then chain this diagram with our earlier diagram (19) and obtain not only a family of parametrizations of  $\mathcal{A}_m$  by Hermitian matrices, but also a rule for passing between the different parametrizations. We will discuss this more thoroughly in the next section.

Due to (25), another appropriate name for the Weyl matrix might have been the ‘‘transfer matrix.’’ In any case it is not surprising that we have a counterpart of Proposition 3.21 for Weyl matrices:

**Proposition 3.33.** *Let  $\lambda, \mu, \eta \in \rho(A) \cap \mathbb{R}$ . Then*

(i)  $\mathbf{M}(\lambda, \lambda) = \mathbf{0}$ ;

$$(ii) \mathbf{M}(\eta, \mu) + \mathbf{M}(\mu, \lambda) = \mathbf{M}(\eta, \lambda);$$

$$(iii) \mathbf{M}(\mu, \lambda) = -\mathbf{M}(\lambda, \mu).$$

*Proof.*

(i) Take  $\mu = \lambda$  in Lemma 3.31.

(ii) By Proposition 3.21(ii) and the definition of the Weyl matrix,

$$(\mathbf{M}(\eta, \lambda))_\lambda = M_\lambda(\eta) = \Gamma(\mu, \lambda)M_\mu(\eta) = \Gamma(\mu, \lambda)(\mathbf{M}(\eta, \mu))_\mu,$$

so Theorem 3.32 gives

$$(\mathbf{M}(\eta, \lambda))_\lambda = (\mathbf{M}(\eta, \mu) + \mathbf{M}(\mu, \lambda))_\lambda.$$

Since  $\mathbf{B} \mapsto \mathbf{B}_\lambda$  is an isomorphism the assertion follows.

(iii) Take  $\eta = \lambda$  in (ii) and use (i).

□

We observe that the above properties are similar to those of a definite integral of a function in one real argument, with integration limits from  $\lambda$  to  $\mu$ . This is not a coincidence, as we will soon derive an integral formula for the Weyl matrix.

Recall that we started with an ordered basis  $\mathbb{E}_\mu$  of  $\mathcal{N}_\mu$ , which by gamma compatibility induced an ordered basis  $\mathbb{E}_\lambda$  of  $\mathcal{N}_\lambda$  for every other  $\lambda \in \rho(A) \cap \mathbb{R}$ . Of course, there is no need to stop there: Lemma 3.10(ii) says that  $\gamma_\lambda(z) : \mathcal{N}_\lambda \rightarrow \mathcal{N}_z$  is defined and bijective also for complex  $z \in \rho(A)$ , so we can extend our gamma family  $\mathbb{E}$  to include these additional bases  $\mathbb{E}_z$ . For this reason, we can also extend the Weyl matrix  $\mathbf{M}(z, \lambda)$  to complex values of  $z \in \rho(A)$  (but only in the first argument, as the Weyl function  $M_\lambda$  is only defined for real  $\lambda$ .) Although we will not need this extended notion of gamma family in the sequel, the reason we are now bringing it up is because this extended Weyl matrix is holomorphic in its first argument:

**Theorem 3.34.**  $z \mapsto \mathbf{M}(z, \lambda)$  is holomorphic on  $\rho(A)$ , and

$$\frac{d}{dz} \mathbf{M}(z, \lambda) = (\langle e_z^i, e_{\bar{z}}^j \rangle)_{ij}.$$

*Proof.* This is a reinterpretation of Corollary 3.16 in terms of the Weyl matrix, and the proof is trivial. □

We say that a function defined on an open subset of the real line is *analytic* if it has a (possibly complex) power series expansion at each point in its domain. Similarly, we say that a real matrix-valued function  $x \mapsto \mathbf{B}(x)$  of a single real argument is analytic if each component function  $x \mapsto \mathbf{B}(x)_{ij}$  is analytic.

**Corollary 3.35.**  $\mathbf{M}(\mu, \lambda)$  is analytic on  $\rho(A) \cap \mathbb{R}$  separately in each argument, and

$$\frac{d}{d\mu}\mathbf{M}(\mu, \lambda) = \mathbf{E}(\mu), \quad \frac{d}{d\lambda}\mathbf{M}(\mu, \lambda) = -\mathbf{E}(\lambda).$$

*Proof.* The first derivative follows from the above proposition and the definition of  $\mathbf{E}(\mu)$ . The second derivative follows from the first by using Proposition 3.33(iii).  $\square$

As a consequence of this corollary, we arrive at an integral formula for the Weyl matrix and its sesquilinear form. (The integral is taken componentwise.)

**Proposition 3.36.** Let  $\lambda < \mu$  be such that  $[\lambda, \mu] \subset \rho(A)$ . Then

$$\mathbf{M}(\mu, \lambda) = \int_{\lambda}^{\mu} \mathbf{E}(t) dt$$

and

$$\mathbf{v}^H \mathbf{M}(\mu, \lambda) \mathbf{u} = \int_{\lambda}^{\mu} \langle \mathbf{u}_t, \mathbf{v}_t \rangle dt \quad \text{for all } \mathbf{u}, \mathbf{v} \in \mathbb{C}^m. \quad (26)$$

*Proof.* By the previous corollary and Proposition 3.33(i),

$$\mathbf{M}(\mu, \lambda) = \mathbf{M}(\lambda, \lambda) + \int_{\lambda}^{\mu} \frac{d}{dt} \mathbf{M}(t, \lambda) dt = \int_{\lambda}^{\mu} \mathbf{E}(t) dt.$$

The second integral formula follows from the first together with (24).  $\square$

**Corollary 3.37.** Let  $\lambda < \mu$  be such that  $[\lambda, \mu] \subset \rho(A)$ . Then  $\mathbf{M}(\mu, \lambda)$  is positive definite.

*Proof.* By (26),  $\mathbf{u}^H \mathbf{M}(\mu, \lambda) \mathbf{u} = \int_{\lambda}^{\mu} \|\mathbf{u}_t\|^2 dt > 0$  for all  $\mathbf{u} \in \mathbb{C}^m \setminus \{0\}$ .  $\square$

As yet another corollary, we obtain a mean value theorem.

**Corollary 3.38.** Let  $\lambda < \mu$  be such that  $[\lambda, \mu] \subset \rho(A)$ . For all  $\mathbf{u} \in \mathbb{C}^m$ , there exists  $\theta \in (\lambda, \mu)$  such that  $\langle \mathbf{u}_{\mu}, \mathbf{u}_{\lambda} \rangle = \|\mathbf{u}_{\theta}\|^2$ .

*Proof.* According to Lemma 3.31,  $\mathbf{u}^H \mathbf{M}(\mu, \lambda) \mathbf{u} = (\mu - \lambda) \langle \mathbf{u}_{\mu}, \mathbf{u}_{\lambda} \rangle$ . Now divide by  $\mu - \lambda$  in (26) and use the mean value theorem for integrals.  $\square$

The following definition is commonly used in Sturm-Liouville theory: Let  $f$  be a measurable function on a bounded or unbounded open interval  $(a, b)$ . We say that  $f$  is in  $L^2$  near  $a$  (resp. near  $b$ ) if there exists  $c \in (a, b)$  such that  $f \in L^2(a, c)$  (resp.  $f \in L^2(c, b)$ ).

Recall our assumption that  $A$  is a self-adjoint extension of  $T$  such that  $\rho(A) \cap \mathbb{R}$  is nonempty.

**Proposition 3.39.** Suppose that  $A$  is lower semibounded.

(i)  $\mu \mapsto \mathbf{M}(\mu, \lambda)$  (resp.  $\lambda \mapsto \mathbf{M}(\mu, \lambda)$ ) is strictly increasing (resp. strictly decreasing) on  $(-\infty, \mathfrak{m}(A))$ ;

(ii) The following are equivalent:

- (a)  $A$  is the Friedrichs extension of  $T$ ;
- (b)  $\lim_{\mu \rightarrow -\infty} \mathbf{u}^H \mathbf{M}(\mu, \lambda) \mathbf{u} = -\infty$  for all  $\mathbf{u} \in \mathbb{C}^m \setminus \{0\}$ ;
- (c)  $\lim_{\lambda \rightarrow -\infty} \mathbf{u}^H \mathbf{M}(\mu, \lambda) \mathbf{u} = +\infty$  for all  $\mathbf{u} \in \mathbb{C}^m \setminus \{0\}$ ;
- (d)  $t \mapsto \|\mathbf{u}_t\|$  is not in  $L^2$  near  $-\infty$  for all  $\mathbf{u} \in \mathbb{C}^m \setminus \{0\}$ .

*Proof.*

- (i) By Corollary 3.18,  $\mu \mapsto M_\lambda(\mu) = (\mathbf{M}(\mu, \lambda))_\lambda$  is strictly increasing on the interval  $(-\infty, \mathfrak{m}(A))$ , so Lemma 3.29 gives that  $\mu \mapsto \mathbf{M}(\mu, \lambda)$  is monotonically increasing while the strictness follows from  $\mathbf{B} \mapsto \mathbf{B}_\lambda$  being an isomorphism. The corresponding assertion for  $\lambda \mapsto \mathbf{M}(\mu, \lambda)$  then follows from Proposition 3.33(iii).
- (ii) By (22),  $\langle M_\lambda(\mu) \mathbf{u}_\lambda, \mathbf{u}_\lambda \rangle = \mathbf{u}^H \mathbf{M}(\mu, \lambda) \mathbf{u}$  for all  $\mathbf{u} \in \mathbb{C}^m$ . Thus the equivalence between (a) and (b) is just a restatement of Proposition 3.19. The equivalence between (b) and (c) is a consequence of Proposition 3.33(iii), and finally the equivalence between (c) and (d) is due to the integral formula (26).

□

### 3.6 Weyl primitives and admissible operators

Let  $T$  be a densely defined symmetric operator with finite defect indices  $(m, m)$ , suppose that  $T$  has a self-adjoint extension  $A$  such that  $\rho(A) \cap \mathbb{R}$  is nonempty, let  $\mathcal{J}$  be a nonempty subset of  $\rho(A) \cap \mathbb{R}$ , and let  $\mathbb{E}$  be a gamma family for  $(T, A)$  on  $\mathcal{J}$ . Let as before  $\mathbf{E}(\mu)$  denote the  $\mathbb{E}$ -matrix of the identity operator in  $\mathcal{N}_\mu$ , and let  $\mathbf{M}(\mu, \lambda)$  denote the Weyl matrix.

Let  $U$  be a connected subset of  $\mathcal{J}$ . If  $\mu \mapsto \mathbf{W}(\mu)$  is any componentwise primitive of  $\mu \mapsto \mathbf{E}(\mu)$  on  $U$ , then Proposition 3.36 implies that

$$\mathbf{W}(\mu) - \mathbf{W}(\lambda) = \mathbf{M}(\mu, \lambda) \quad \text{for all } \lambda, \mu \in U.$$

Conversely, if a family  $\{\mathbf{W}(\mu) : \mu \in U\}$  of matrices satisfies the above identity, then Corollary 3.35 implies that  $\mu \mapsto \mathbf{W}(\mu)$  is analytic with derivative

$$\mathbf{W}'(\mu) = \frac{\partial}{\partial \mu} \mathbf{M}(\mu, \lambda) = \mathbf{E}(\mu) \quad \text{for all } \mu \in U.$$

This motivates our next definition.

**Definition 3.40.** A *Weyl primitive* for  $\mathbb{E}$  is a family  $\mathbf{W} = \{\mathbf{W}(\mu) : \mu \in \mathcal{J}\}$  of Hermitian  $m \times m$  matrices such that

$$\mathbf{W}(\mu) - \mathbf{W}(\lambda) = \mathbf{M}(\mu, \lambda) \quad \text{for all } \lambda, \mu \in \mathcal{J}. \quad (27)$$

As a first example, note that  $\mu \mapsto \mathbf{M}(\mu, \lambda)$  itself is a Weyl primitive for  $\mathbb{E}$  by Proposition 3.33. Since any Weyl primitive is analytic with derivative  $\mu \mapsto \mathbf{E}(\mu)$ , we see that on each connected subset of  $\mathcal{J}$  any two Weyl primitives may differ by at most a constant Hermitian matrix. In particular, if  $\mathcal{J}$  is connected, then each Weyl primitive is of the form  $\mu \mapsto \mathbf{M}(\mu, \lambda) + \mathbf{B}$  for some constant Hermitian matrix  $\mathbf{B}$ .

As an immediate consequence of the definition, Corollary 3.35, and Proposition 3.39, we have

**Proposition 3.41.** *Let  $\mathbf{W}$  be a Weyl primitive for  $\mathbb{E}$ . Then  $\mu \mapsto \mathbf{W}(\mu)$  is strictly increasing and analytic with derivative  $\mathbf{W}'(\mu) = \mathbf{E}(\mu)$ . Furthermore,  $A$  is the Friedrichs extension of  $T$  if and only if*

$$\lim_{\mu \rightarrow -\infty} \mathbf{u}^H \mathbf{W}(\mu) \mathbf{u} = -\infty \quad \text{for all } \mathbf{u} \in \mathbb{C} \setminus \{0\}.$$

In order to avoid repeating the same list of assumptions every time we wish to use the theory in this and the previous sections, let us introduce the following terminology:

**Definition 3.42.** An *admissible operator* is a triplet  $(T, \mathbb{E}, \mathbf{W})$  consisting of

- (i) a densely defined lower semibounded operator  $T$  with finite defect indices;
- (ii) a gamma family  $\mathbb{E}$  for  $(T, T_F)$  on  $(-\infty, \mathbf{m}(T))$ , where  $T_F$  is the Friedrichs extension of  $T$ ;
- (iii) a Weyl primitive  $\mathbf{W} = \{\mathbf{W}(\mu) : \mu < \mathbf{m}(T)\}$  for  $\mathbb{E}$ .

The word “admissible” (in Swedish: ”tillåten”) is meant in the sense of “admissible for the purposes of this thesis” and was chosen for its neutral tone, so as to not imply that admissible operators are mathematical objects of interest outside of this thesis. In the definition, we have assumed  $A = T_F$ , as this is the only case we will encounter in practice. Note that this implies that the Weyl primitive  $\mathbf{W}$  satisfies the last assertion of Proposition 3.41. Finally, we would like to point out that if  $(T, \mathbb{E}, \mathbf{W})$  is an admissible operator, then it follows from Proposition 2.10 that  $T$  has defect indices  $(m, m)$  if and only if  $m$  is exactly the cardinality of each base in  $\mathbb{E}$ .

We now state a “master theorem” for admissible operators that describes some of the self-adjoint extensions of the operator in the triplet. For this purpose, recall Lemma 3.3 and more specifically the definition of the sets  $\mathcal{A}_n$ . Recall also that  $U_\lambda : \mathbb{C}^m \rightarrow \mathcal{N}_\lambda$  denotes the isomorphism that maps  $\mathbf{u} \in \mathbb{C}^m$  onto  $\mathbf{u}_\lambda := \sum_i \mathbf{u}_i e_\lambda^i \in \mathcal{N}_\lambda$ , where  $\mathbb{E}_\lambda = (e_\lambda^1, \dots, e_\lambda^m)$  is the basis of  $\mathcal{N}_\lambda$ .

**Theorem 3.43.** *Let  $(T, \mathbb{E}, \mathbf{W})$  be an admissible operator and let  $(m, m)$  be the defect indices of  $T$ . Then, for all  $\lambda < \mathbf{m}(T)$ ,*

- (i) *there exists a bijection  $\mathcal{M}_{sa}(m) \rightarrow \mathcal{A}_m$ , where the extension  $T_{\mathbf{B}} \in \mathcal{A}_m$  associated to  $\mathbf{B} \in \mathcal{M}_{sa}(m)$  has domain*

$$\mathcal{D}(T_{\mathbf{B}}) = \{u = f + (T_F - \lambda)^{-1}(\mathbf{B} - \mathbf{W}(\lambda))_\lambda \mathbf{u}_\lambda + \mathbf{u}_\lambda : f \in \mathcal{D}(\overline{T}), \mathbf{u} \in \mathbb{C}^m\}$$

and action

$$T_{\mathbf{B}}u = \bar{T}f + (I + (T_F - \lambda)^{-1})(\mathbf{B} - \mathbf{W}(\lambda))_{\lambda} \mathbf{u}_{\lambda} + \lambda \mathbf{u}_{\lambda}$$

and is independent of  $\lambda$ .

(ii) the quadratic form of  $T_{\mathbf{B}}$  has domain

$$\mathcal{D}[T_{\mathbf{B}}] = \mathcal{D}[T_F] \dot{+} \mathcal{N}_{\lambda}$$

and action

$$T_{\mathbf{B}}[f + \mathbf{u}_{\lambda}] = T_F[f] + \mathbf{u}^H(\mathbf{B} - \mathbf{W}(\lambda))\mathbf{u} + \lambda(\|f + \mathbf{u}_{\lambda}\|^2 - \|f\|^2)$$

for  $f \in \mathcal{D}[T_F]$ ,  $\mathbf{u} \in \mathbb{C}^m$ ;

(iii)  $T_{\mathbf{B}} \geq \lambda$  if and only if  $\mathbf{B} \geq \mathbf{W}(\lambda)$ ;

(iv)  $\mathcal{N}(T_{\mathbf{B}} - \lambda) = U_{\lambda}\mathcal{N}(\mathbf{B} - \mathbf{W}(\lambda))$ .

*Proof.*

(i) Let  $\lambda, \mu < \mathfrak{m}(T)$ . It follows from (27) that

$$(\mathbf{B} - \mathbf{W}(\mu)) + \mathbf{M}(\mu, \lambda) = \mathbf{B} - \mathbf{W}(\lambda) \quad \text{for all } \mathbf{B} \in \mathcal{M}_{sa}(m),$$

which can be expressed as the following commutative diagram:

$$\begin{array}{ccc} & & \mathcal{M}_{sa}(m) \\ \mathbf{B} \mapsto \mathbf{B} - \mathbf{W}(\mu) & \nearrow & \\ \mathcal{M}_{sa}(m) & & \downarrow \mathbf{B} \mapsto \mathbf{B} + \mathbf{M}(\mu, \lambda) \\ \mathbf{B} \mapsto \mathbf{B} - \mathbf{W}(\lambda) & \searrow & \mathcal{M}_{sa}(m) \end{array}$$

Upon chaining this diagram with (19) and (25) we obtain another commutative diagram

$$\begin{array}{ccccc} & & \mathcal{M}_{sa}(m) & \xrightarrow{\sim} & \mathcal{B}_{sa}(\mathcal{N}_{\mu}) \\ \mathbf{B} \mapsto \mathbf{B} - \mathbf{W}(\mu) & \nearrow & \downarrow \mathbf{B} \mapsto \mathbf{B} + \mathbf{M}(\mu, \lambda) & & \downarrow \Gamma(\mu, \lambda) \\ \mathcal{M}_{sa}(m) & & & & \mathcal{A}_m \\ \mathbf{B} \mapsto \mathbf{B} - \mathbf{W}(\lambda) & \searrow & \mathcal{M}_{sa}(m) & \xrightarrow{\sim} & \mathcal{B}_{sa}(\mathcal{N}_{\lambda}) \\ & & & & \uparrow T_{\cdot}^{\lambda} \end{array} \quad (28)$$

in which every map is a bijection. Hence, for each  $\mathbf{B} \in \mathcal{M}_{sa}(m)$  there exists an associated self-adjoint extension  $T_{(\mathbf{B} - \mathbf{W}(\lambda))_{\lambda}}^{\lambda} \in \mathcal{A}_m$ , which by

the commutativity of the above diagram is independent of  $\lambda < \mathfrak{m}(T)$ . We therefore have a well-defined parametrization of  $\mathcal{A}_m$  by Hermitian matrices through the map

$$\mathbf{B} \mapsto T_{\mathbf{B}} := T_{(\mathbf{B} - \mathbf{W}(\lambda))_\lambda}^\lambda \quad \text{for all } \mathbf{B} \in \mathcal{M}_{sa}(m). \quad (29)$$

The expressions for the domain and action follow from Theorem 3.1.

- (ii) With notation as in (29), Theorem 3.2(ii) implies that  $T_{\mathbf{B}} \geq \lambda$  if and only if  $(\mathbf{B} - \mathbf{W}(\lambda))_\lambda \geq 0$ , which by Lemma 3.29(ii) is equivalent to  $\mathbf{B} - \mathbf{W}(\lambda) \geq \mathbf{0}$ .
- (iii) The assertion follows in a straightforward manner from Theorem 3.2(i); we only have to note that  $\mathcal{D}[(\mathbf{B} - \mathbf{W}(\lambda))_\lambda] = \mathcal{N}_\lambda$  and that (22) implies  $(\mathbf{B} - \mathbf{W}(\lambda))_\lambda[\mathbf{u}_\lambda] = \mathbf{u}^H(\mathbf{B} - \mathbf{W}(\lambda))\mathbf{u}$  for all  $\mathbf{u} \in \mathbb{C}^m$ .
- (iv) [28, Proposition 14.17(i)] implies that

$$\mathcal{N}(T_{\mathbf{B}} - \lambda) = \gamma_\lambda(\lambda) \mathcal{N}((\mathbf{B} - \mathbf{W}(\lambda))_\lambda - M_\lambda(\lambda))$$

and Proposition 3.13 gives that the right-hand side reduces to

$$\mathcal{N}((\mathbf{B} - \mathbf{W}(\lambda))_\lambda)$$

which is equal to

$$U_\lambda \mathcal{N}(\mathbf{B} - \mathbf{W}(\lambda))$$

as can be seen by taking  $z = 0$  in Lemma 3.29(i). □

The parametrization in (i) is unfortunately far from unique, since it depends on both the choice of gamma basis and the choice of Weyl primitive. However, in the application we have in mind (Section 4.4), there will exist natural choices for each of these, so the lack of uniqueness will not pose an issue.

**Theorem 3.44.** *Let  $(T, \mathbb{E}, \mathbf{W})$  be an admissible operator and let  $(m, m)$  be the defect indices of  $T$ . Let  $\mathbf{B} \in \mathcal{M}_{sa}(m)$  and  $\lambda < \mathfrak{m}(T)$ . Then*

$$\mathfrak{m}(T_{\mathbf{B}}) = \lambda \quad \text{if and only if} \quad \lambda_{\max}(\mathbf{W}(\lambda) - \mathbf{B}) = 0.$$

*Proof.* If  $\mathfrak{m}(T_{\mathbf{B}}) = \lambda$ , then Proposition 2.11 implies that  $\lambda$  is an eigenvalue of  $T_{\mathbf{B}}$ . Thus  $\mathfrak{m}(T_{\mathbf{B}}) = \lambda$  if and only if

$$\mathcal{N}(T_{\mathbf{B}} - \lambda) \neq \{0\} \quad \text{and} \quad T_{\mathbf{B}} \geq \lambda.$$

By Theorem 3.43(iii-vi), this holds if and only if

$$\mathcal{N}(\mathbf{W}(\lambda) - \mathbf{B}) \neq \{0\} \quad \text{and} \quad 0 \geq \mathbf{W}(\lambda) - \mathbf{B},$$

which in turn is equivalent to  $\lambda_{\max}(\mathbf{W}(\lambda) - \mathbf{B}) = 0$ . □

### 3.7 Special case: Defect indices $(1, 1)$

Let  $(T, \mathbb{E}, \mathbf{W})$  be an admissible operator and assume that  $T$  has defect indices  $(1, 1)$ . We shall now proceed to prove some results about such admissible operators which will later be used in Section 5.1.

As we remarked in Section 3.6, the defect indices of  $T$  being  $(1, 1)$  is equivalent to each basis in the gamma family having cardinality 1:

$$\mathbb{E} = \{\mathbb{E}_\lambda : \lambda < \mathbf{m}(T)\} = \{(e_\lambda) : \lambda < \mathbf{m}(T)\}.$$

Lemma 3.3 and Theorem 3.43(i) imply that the set of all self-adjoint extensions of  $T$  is the disjoint union

$$\mathcal{A}_0 \cup \mathcal{A}_1 = \{T_F\} \cup \{T_{\mathbf{B}} : \mathbf{B} \in \mathcal{M}_{sa}(1)\}.$$

In particular, *every* non-Friedrichs extension of  $T$  is of the form specified by Theorem 3.43(i). Of course, each matrix in  $\mathcal{M}_{sa}(1)$  is just a scalar matrix  $\alpha \mathbf{I}$  for some  $\alpha \in \mathbb{R}$ . It is then convenient to use the shorthand

$$T_\alpha := T_{\alpha \mathbf{I}}, \quad \text{for } \alpha \in \mathbb{R}.$$

Proposition 2.11 implies that  $\sigma(T_\alpha) \cap (-\infty, \mathbf{m}(T))$  is either empty or consists of at most a single isolated simple eigenvalue. Recall now that  $\mathbf{m}(T_\alpha) = \min \sigma(T_\alpha)$ , and moreover  $\mathbf{m}(T_\alpha) \leq \mathbf{m}(T)$  since  $T_\alpha$  is an extension of  $T$  (see Section 2.5). It follows that for each  $\alpha \in \mathbb{R}$  there is one of two mutually exclusive alternatives:

**Case 1:**  $\mathbf{m}(T_\alpha) = \mathbf{m}(T)$  and  $\sigma(T_\alpha) \cap (-\infty, \mathbf{m}(T)) = \emptyset$ ;

**Case 2:**  $\mathbf{m}(T_\alpha) < \mathbf{m}(T)$  and  $\sigma(T_\alpha) \cap (-\infty, \mathbf{m}(T)) = \{\mathbf{m}(T_\alpha)\}$  and  $\mathbf{m}(T_\alpha)$  is a simple eigenvalue.

As for the Weyl primitive, we have  $\mathbf{W}(\lambda) = \mathbf{w}(\lambda) \mathbf{I}$  for all  $\lambda < \mathbf{m}(T)$  and some scalar function  $\mathbf{w} : (-\infty, \mathbf{m}(T)) \rightarrow \mathbb{R}$ . Proposition 3.41 yields that  $\mathbf{w}$  is strictly increasing, analytic with derivative  $\mathbf{w}'(\lambda) = \langle e_\lambda, e_\lambda \rangle = \|e_\lambda\|^2$ , and

$$\lim_{\lambda \rightarrow -\infty} \mathbf{w}(\lambda) = -\infty.$$

It follows that  $\mathbf{w} : (-\infty, \mathbf{m}(T)) \rightarrow \mathbb{R}$  is a bijection if and only if the limit

$$\mathbf{w}(T) := \lim_{\lambda \nearrow \mathbf{m}(T)} \mathbf{w}(\lambda)$$

is equal to  $+\infty$ . We observe that if  $\mathbf{w}(T) = +\infty$  for one choice of Weyl primitive, then it is true for all choices, as any other Weyl primitive must be of the form  $\mathbf{w} + c$  for some constant  $c \in \mathbb{R}$ . In fact, this property is even independent of the gamma family: Choosing another gamma family amounts (by gamma compatibility) to rescaling each basis vector  $e_\lambda$  by a fixed nonzero (complex) constant, and the identity  $\mathbf{w}(\mu) - \mathbf{w}(\lambda) = \int_\lambda^\mu \|e_t\|^2 dt$  implies that this rescaling cannot affect whether the above limit diverges or not. In other words, the question of whether  $\mathbf{w}(T) = +\infty$  or not is only dependent on the operator  $T$  itself and not on the particular choice of admissible operator.

**Proposition 3.45.** *Let  $\alpha \in \mathbb{R}$ . Then  $\mathfrak{m}(T_\alpha) < \mathfrak{m}(T)$  if and only if  $\alpha < \mathfrak{w}(T)$ . Letting  $\mathfrak{m}(\alpha) := \mathfrak{m}(T_\alpha)$ , we have that the two maps*

$$\mathfrak{w} : (-\infty, \mathfrak{m}(T)) \rightarrow (-\infty, \mathfrak{w}(T)) \quad \text{and} \quad \mathfrak{m} : (-\infty, \mathfrak{w}(T)) \rightarrow (-\infty, \mathfrak{m}(T))$$

*are inverses of each other.*

*Proof.* Let  $\lambda < \mathfrak{m}(T)$ . Since the largest eigenvalue of a matrix of size  $1 \times 1$  is equal to the only component of the matrix, Theorem 3.44 implies that

$$\mathfrak{m}(\alpha) = \lambda \quad \text{if and only if} \quad \mathfrak{w}(\lambda) = \alpha.$$

Thus, if case 1 holds then  $\mathfrak{w}(\lambda) \neq \alpha$ , and since  $\mathfrak{w}$  is a bijection onto  $(-\infty, \mathfrak{w}(T))$  we must therefore have  $\alpha \geq \mathfrak{w}(T)$ . If case 2 holds, then  $\alpha = \mathfrak{w}(\mathfrak{m}(\alpha)) < \mathfrak{w}(T)$ . This proves the first assertion. The second assertion then follows from the above equivalence.  $\square$

There is an interesting connection between the extended real number  $\mathfrak{w}(T)$  and a recent result [15]. For it has been shown [15, Theorem 2.6] that if  $S$  is a densely defined lower semibounded symmetric operator, then  $S$  has a lower semibounded self-adjoint extension  $S_{LT}$ , the “least-top extension”, such that for any lower semibounded self-adjoint extension  $A$  of  $S$ ,

$$\mathfrak{m}(A) = \mathfrak{m}(S) \quad \text{if and only if} \quad A \geq S_{LT}.$$

Let  $\alpha \in \mathbb{R}$ . Now, on the one hand Proposition 3.45 asserts that

$$\mathfrak{m}(T_\alpha) = \mathfrak{m}(T) \quad \text{if and only if} \quad \alpha \geq \mathfrak{w}(T)$$

while on the other hand, Theorem 3.43(ii) (more specifically, our expression for the quadratic forms) implies that  $T_\alpha \geq T_{\mathfrak{w}(T)}$  if and only if  $\alpha \geq \mathfrak{w}(T)$ . From this we conclude that  $T_{LT} = T_{\mathfrak{w}(T)}$ .

**Corollary 3.46.** *The map  $\mathfrak{m} : (-\infty, \mathfrak{w}(T)) \rightarrow (-\infty, \mathfrak{m}(T))$  is a strictly increasing and analytic bijection with derivative  $\mathfrak{m}'(\alpha) = 1 / \|e_{\mathfrak{m}(\alpha)}\|^2$ .*

*Proof.* Since  $\mathfrak{w}$  is a strictly increasing and analytic bijection, its inverse  $\mathfrak{m}$  must also be a strictly increasing and analytic bijection. By  $\mathfrak{w}'(\lambda) = \|e_\lambda\|^2$  along with the well-known formula for the derivative of an inverse, we have

$$\mathfrak{m}'(\alpha) = \frac{d}{d\alpha} \mathfrak{w}^{-1}(\alpha) = \frac{1}{\mathfrak{w}'(\mathfrak{w}^{-1}(\alpha))} = \frac{1}{\|e_{\mathfrak{m}(\alpha)}\|^2}.$$

$\square$

**Lemma 3.47.** *The following are equivalent:*

- (i)  $\mathfrak{m}(T_\alpha) < \mathfrak{m}(T)$  for all  $\alpha \in \mathbb{R}$ ;
- (ii)  $\mathfrak{w}(T) = +\infty$ ;
- (iii)  $t \mapsto \|e_t\|$  is not in  $L^2$  near  $\mathfrak{m}(T)$ .

*Proof.* Proposition 3.45 provides the equivalence between (i) and (ii), as it implies that (i) holds exactly if  $\alpha < \mathfrak{w}(T)$  for all  $\alpha \in \mathbb{R}$ . The equivalence between (ii) and (iii) follows from the identity  $\mathfrak{w}(\mu) - \mathfrak{w}(\lambda) = \int_\lambda^\mu \|e_t\|^2 dt$ .  $\square$

## 4 Point-interaction Hamiltonians

We shall now begin our study of point-interaction Hamiltonians in bounded domains. Section 4.1 starts with an overview of distributions and Sobolev spaces. These concepts are then immediately applied in Section 4.2, in which we construct the Dirichlet Laplacian as the Friedrichs extension of a certain densely defined lower semibounded operator in  $L^2(\Omega)$ . Section 4.3 introduces an important function associated to the Dirichlet Laplacian called the Green's function. Using the above self-adjoint extension theory, we then proceed to construct the point-interaction Hamiltonians and investigate their spectral properties in Sections 4.4 and 4.5, respectively.

Throughout this entire section, let  $\Omega$  denote a nonempty open subset of  $\mathbb{R}^d$ ,  $d \geq 1$ . We say that  $\Omega$  is *bounded* if it is contained in some open ball. The *boundary* of  $\Omega$  is the closed set  $\partial\Omega := \overline{\Omega} \setminus \Omega$ . If  $\Omega$  is bounded and  $k$  a nonnegative integer, then we say that  $\Omega$  *has  $C^k$ -boundary* if the following holds: For any  $x \in \partial\Omega$  there exists a neighbourhood  $U$  of  $x$  and a function  $f \in C^k(\mathbb{R}^{d-1}, \mathbb{R})$  such that—upon relabeling and reorienting the coordinate axes if necessary—we have

$$\Omega \cap U = \{(x_1, \dots, x_d) \in U : x_d > f(x_1, \dots, x_{d-1})\}.$$

If  $k \geq 1$ , then the *surface measure* of the piece  $\partial\Omega \cap U$  is defined as

$$\sigma(\partial\Omega \cap U) := \int_{\{x \in \mathbb{R}^{d-1} : (x, f(x)) \in U\}} \sqrt{\det(J(f)^T J(f))} dx$$

where  $J(f)$  is the Jacobian matrix of  $f$ . This induces a measure  $\sigma$  on  $\partial\Omega$  which is again called the *surface measure* of  $\partial\Omega$ . The associated  $L^2$ -space of complex-valued functions on  $\partial\Omega$ , square-integrable with respect to the surface measure, will be denoted  $L^2(\partial\Omega)$ . Still supposing  $k \geq 1$ , the *outward unit normal vector* at  $x = (x_1, \dots, x_d) \in \partial\Omega \cap U$  is defined as

$$\nu(x) := \frac{(-\nabla f(x_1, \dots, x_{d-1}), 1)}{\sqrt{|\nabla f(x_1, \dots, x_{d-1})|^2 + 1}}$$

or, if the coordinate axes have been relabeled and/or reoriented,  $\nu(x)$  is defined as the result of applying the opposite sequence of transformations to the right-hand side. (Both the surface measure and the outward unit normal vector are of course independent of the particular choice of  $f$ .)

### 4.1 Distributions and Sobolev spaces

For any bounded complex-valued function  $f$  defined on a subset of  $\mathbb{R}^d$ , let

$$\|f\|_\infty := \sup |f(x)|,$$

where the supremum is taken over the domain of  $f$ . Let  $C_0^\infty(\Omega)$  denote the normed space of smooth complex-valued functions on  $\Omega$  with compact support

and norm given by  $\varphi \mapsto \|\varphi\|_\infty$ . Let

$$L^2(\Omega) := \left\{ f : \Omega \rightarrow \mathbb{C} : f \text{ is measurable and } \int_\Omega |f|^2 dx < +\infty \right\}$$

where the integral is taken in the Lebesgue sense, and recall that  $L^2(\Omega)$  is a Hilbert space with inner product

$$\langle f, g \rangle := \int_\Omega f \bar{g} dx \quad \text{for } f, g \in L^2(\Omega).$$

(See, e.g., [14, Section 3.2].) The induced norm on  $L^2(\Omega)$  will be denoted  $\|\cdot\|$ .

**Lemma 4.1** ([19, Theorem 1.2.5]).  $C_0^\infty(\Omega)$  is dense in  $(L^2(\Omega), \|\cdot\|)$ .

A *multi-index* is a vector  $\alpha = (\alpha_1, \dots, \alpha_d)$  of nonnegative integers. For any multi-index  $\alpha$ , let

$$|\alpha| := \alpha_1 + \dots + \alpha_d \quad \text{and} \quad \partial^\alpha := \left( \frac{\partial}{\partial x_1} \right)^{\alpha_1} \dots \left( \frac{\partial}{\partial x_d} \right)^{\alpha_d}.$$

A *distribution* on  $\Omega$  is a linear functional  $T : C_0^\infty(\Omega) \rightarrow \mathbb{C}$  such that for every compact subset  $K \subset \Omega$  there exist a positive constant  $C_K$  and a nonnegative integer  $n_K$  such that

$$|T\varphi| \leq C_K \sum_{|\alpha| \leq n_K} \|\partial^\alpha \varphi\|_\infty \quad \text{for all } \varphi \in C_0^\infty(\Omega), \text{ supp } \varphi \subset K.$$

The set of distributions on  $\Omega$  form a complex vector space.

An important class of distributions is the class of Dirac delta distributions  $\delta_x$  for  $x \in \Omega$ . They are defined by  $\delta_x \varphi = \varphi(x)$  for all  $\varphi \in C_0^\infty(\Omega)$ .

**Lemma 4.2.**  $\{\delta_x : x \in \Omega\}$  is a linearly independent set in the vector space of distributions.

By this we mean that each finite subset of  $\{\delta_x : x \in \Omega\}$  is a linearly independent set in the usual sense.

*Proof.* Let  $X$  be a finite subset of  $\Omega$  and suppose  $\sum_{x \in X} c_x \delta_x = 0$  for some  $c_x \in \mathbb{C}$ . Let  $x_0 \in X$ . Let  $B$  be an open ball centered at  $x_0$  and small enough that  $B \cap X = \{x_0\}$ . Choose  $\varphi \in C_0^\infty(B)$  such that  $\varphi(x_0) = 1$ . By applying both sides of our distributional equality to  $\varphi$  we obtain  $0 = \sum_x c_x \varphi(x) = c_{x_0}$ . Thus all coefficients  $c_x$  are zero, and  $\{\delta_x : x \in X\}$  is a linearly independent set.  $\square$

Any  $f \in L^2(\Omega)$  induces a distribution  $T_f$  on  $\Omega$  by

$$T_f \varphi := \int_\Omega f \varphi dx = \langle f, \bar{\varphi} \rangle \quad \text{for all } \varphi \in C_0^\infty(\Omega).$$

If  $f, g \in L^2(\Omega)$  and  $T_f = T_g$ , then Lemma 4.1 implies  $f = g$ . Thus we have a linear embedding  $f \mapsto T_f$ , and we may in this sense say that we have the inclusions

$$C_0^\infty(\Omega) \subset L^2(\Omega) \subset \{\text{distributions on } \Omega\}. \quad (30)$$

**Lemma 4.3.**  $\delta_x$  is not of the form  $T_f$  for any  $f \in L^2(\Omega)$ .

*Proof.* Suppose that  $\delta_x = T_f$  for some  $f \in L^2(\Omega)$ . Take  $\varphi \in C_0^\infty(\Omega)$  supported on the unit ball such that  $0 \leq \varphi(x) \leq 1$  for  $|x| \leq 1$  and  $\varphi(0) = 1$ , and let  $\varphi_n(x) = \varphi(nx)$  for  $n \in \mathbb{N}$ . Hence  $|f\varphi_n| \leq |f|$  pointwise for all  $n$  and  $f\varphi_n \rightarrow 0$  almost everywhere, so  $\int_\Omega f\varphi_n dx \rightarrow 0$  by the dominated convergence theorem. But this is a contradiction, since  $\int_\Omega f\varphi_n dx = T_f\varphi_n = \delta_x\varphi_n = 1$  for all  $n$ .  $\square$

Let  $T$  be a distribution on  $\Omega$ . For any multi-index  $\alpha$ , the *distributional derivative*  $\partial^\alpha T$  is defined by

$$(\partial^\alpha T)\varphi := (-1)^{|\alpha|} T(\partial^\alpha \varphi) \quad \text{for all } \varphi \in C_0^\infty(\Omega)$$

and is again a distribution on  $\Omega$  [19, Section 3.1]. By using partial integration, one can show [10, Section 5.2.1] that  $\partial^\alpha T_\varphi = T_{\partial^\alpha \varphi}$  for any  $\varphi \in C_0^\infty(\Omega)$  and multi-index  $\alpha$ . Thus we have a notion of derivative on the largest set in (30) that agrees with our classical notion on the smallest. In particular, we can “differentiate” functions in  $L^2(\Omega)$  arbitrarily many times, though the result will in general only be a distribution.

Let  $f \in L^2(\Omega)$  and let  $\alpha$  be a multi-index. We say that  $f$  has a *weak derivative of order  $\alpha$*  if  $\partial^\alpha T_f = T_g$  for some (necessarily unique)  $g \in L^2(\Omega)$ . In this case  $\partial^\alpha f := g$  is called the *weak derivative of  $f$  of order  $\alpha$* . Note that the weak derivative of  $f$  of order  $(0, 0, \dots, 0)$  is just  $f$  itself. Given a nonnegative integer  $k$ , we define the *Sobolev space of order  $k$*  as the vector space

$$H^k(\Omega) := \{f \in L^2(\Omega) : f \text{ has a weak derivative of order } \alpha \text{ for all } |\alpha| \leq k\},$$

and we equip  $H^k(\Omega)$  with the inner product

$$\langle f, g \rangle_{H^k(\Omega)} := \sum_{|\alpha| \leq k} \langle \partial^\alpha f, \partial^\alpha g \rangle_{L^2(\Omega)} \quad \text{for all } f, g \in H^k(\Omega)$$

which induces the norm

$$\|f\|_{H^k(\Omega)}^2 := \sum_{|\alpha| \leq k} \|\partial^\alpha f\|_{L^2(\Omega)}^2 \quad \text{for all } f \in H^k(\Omega)$$

One can show that  $(H^k(\Omega), \langle \cdot, \cdot \rangle_{H^k(\Omega)})$  is a Hilbert space [10, Section 5.2.3]. Note that  $H^0(\Omega) = L^2(\Omega)$ , not just as sets but as Hilbert spaces. Finally, we define  $H_0^k(\Omega)$  as the closure of  $C_0^\infty(\Omega)$  in  $(H^k(\Omega), \langle \cdot, \cdot \rangle_{H^k(\Omega)})$ , which automatically makes it a Hilbert space.

Any  $f \in H^1(\Omega)$  has a well-defined gradient  $\nabla f := (\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_d})$ , where

$$|\nabla f|^2 = \sum_{i=1}^d \left| \frac{\partial f}{\partial x_i} \right|^2$$

is integrable, and

$$\|\nabla f\|^2 = \sum_{i=1}^d \left\| \frac{\partial f}{\partial x_i} \right\|^2.$$

Since this quantity appears often we will use the shorthand  $\|\nabla f\| := \|\nabla f\|$ . Note in particular that

$$\|f\|_{H^1(\Omega)}^2 = \sum_{|\alpha| \leq 1} \|\partial^\alpha f\|^2 = \|f\|^2 + \|\nabla f\|^2. \quad (31)$$

**Proposition 4.4** ([10, Section 5.6]). *Suppose  $\Omega$  is bounded. Then*

- (i) *the embedding  $(H_0^1(\Omega), \|\cdot\|_{H^1(\Omega)}) \rightarrow (L^2(\Omega), \|\cdot\|)$  is compact;*
- (ii) *there exists a positive constant  $c_\Omega$  such that Poincaré's inequality holds:*

$$c_\Omega \|f\|^2 \leq \|\nabla f\|^2 \quad \text{for all } f \in H_0^1(\Omega).$$

Under some mild regularity assumptions on  $\Omega$ , the next theorem makes it possible to assign boundary values along  $\partial\Omega$  to functions in  $H^1(\Omega)$ .

**Theorem 4.5** ([10, Section 5.5, Theorems 1 and 2]). *Suppose  $\Omega$  is bounded with  $C^1$ -boundary. Then there exists a unique bounded linear operator*

$$\text{Tr} : (H^1(\Omega), \|\cdot\|_{H^1(\Omega)}) \rightarrow (L^2(\partial\Omega), \|\cdot\|_{L^2(\partial\Omega)})$$

*such that  $\text{Tr}(f) = f \upharpoonright \partial\Omega$  for all  $f \in H^1(\Omega) \cap C(\overline{\Omega})$ . Moreover,  $H_0^1(\Omega) = \mathcal{N}(\text{Tr})$ .*

The operator  $\text{Tr}$  is called the *trace operator*, and for any  $f \in H^1(\Omega)$  the associated “boundary value”  $\text{Tr}(f) \in L^2(\partial\Omega)$  is called the *trace* of  $f$ .

The following proposition is a special case of the Sobolev embedding theorem [10, Theorem II.6.6]. (We actually have the stronger statement that  $H^2(\Omega)$  embeds continuously into the Hölder space  $C^{2,\gamma}(\overline{\Omega})$  for a certain  $0 < \gamma < 1$  depending on  $d$ , but we will not need this strengthened version.)

**Proposition 4.6.** *Suppose  $d \leq 3$  and  $\Omega$  is bounded with  $C^1$ -boundary. Then  $H^2(\Omega) \subset C(\overline{\Omega})$ , and there exists a positive constant  $c$  such that*

$$\sup_{x \in \overline{\Omega}} |f(x)| \leq c \|f\|_{H^2(\Omega)} \quad \text{for all } f \in H^2(\Omega).$$

We end this section with a couple of lemmas. These will be used in Section 4.4 to prove that a certain linear operator  $H$  is closed.

**Lemma 4.7.** *Let  $k \geq 0$  be an integer such that  $2k + 1 \leq d$ . Let  $\varphi \in C_0^\infty(\mathbb{R}^d)$ , and let  $\varphi_n(x) = \varphi(nx)$  for  $n \geq 1$ . Then  $\|\varphi_n\|_{H^k(\mathbb{R}^d)} \rightarrow 0$  as  $n \rightarrow \infty$ .*

*Proof.* For any multi-index  $\alpha$ ,

$$(\partial^\alpha \varphi_n)(x) = n^{|\alpha|} (\partial^\alpha \varphi)(nx)$$

and

$$|(\partial^\alpha \varphi_n)(x)|^2 = n^{2|\alpha|} |(\partial^\alpha \varphi)(nx)|^2$$

so integrating both sides over  $\mathbb{R}^d$  yields

$$\|\partial^\alpha \varphi_n\|^2 = n^{2|\alpha|} \int |(\partial^\alpha \varphi)(nx)|^2 dx.$$

The map  $x \mapsto nx$  is a bijection of  $\mathbb{R}^d$  onto itself, and the determinant of the Jacobian of the map is  $n^d$ . Hence, by the change of variables formula for integrals,

$$\|\partial^\alpha \varphi_n\|^2 = n^{2|\alpha|-d} \|\partial^\alpha \varphi\|^2.$$

If  $|\alpha| \leq k$ , then  $2|\alpha| - d \leq -1$ , and summing both sides over all such  $\alpha$  gives

$$\|\varphi_n\|_{H^k}^2 \leq n^{-1} \|\varphi\|_{H^k}^2.$$

Taking  $n \rightarrow \infty$ , the assertion follows.  $\square$

**Lemma 4.8.** *Let  $k$  be as in the previous lemma and let  $X \subset \mathbb{R}^d$  be a finite set. Then the set*

$$\{f \in C_0^\infty(\Omega) : f(x) = 0 \text{ for all } x \in X\} \quad (32)$$

*is dense in  $(H_0^k(\Omega), \|\cdot\|_{H^k(\Omega)})$ .*

*Proof.* Let  $f \in H_0^k(\Omega)$  and let  $\epsilon > 0$ . By definition of  $H_0^k(\Omega)$ , we can find  $\varphi \in C_0^\infty(\Omega)$  such that  $\|f - \varphi\|_{H^k(\Omega)} < \epsilon/2$ . Let  $\psi \in C_0^\infty(\mathbb{R}^d)$  be such that  $\psi(0) = 1$ , and let  $\psi_n(x) = \psi(nx)$  for  $n \geq 1$ . By the previous lemma,  $\|\psi_n\|_{H^k(\mathbb{R}^d)} \rightarrow 0$  as  $n \rightarrow \infty$ . For all large enough  $n$ , the function

$$\varphi_n(x) = \varphi(x) - \sum_{x_0 \in X} \varphi(x_0) \psi_n(x - x_0)$$

is in (32). Moreover,  $\|\varphi - \varphi_n\|_{H^k(\Omega)} \rightarrow 0$  as  $n \rightarrow \infty$ . Hence we can choose  $N$  such that  $\|\varphi - \varphi_N\|_{H^k(\Omega)} < \epsilon/2$ , and then  $\|f - \varphi_N\|_{H^k(\Omega)} < \epsilon$  by the triangle inequality. This shows that every function in  $H_0^k(\Omega)$  can be approximated arbitrarily well in  $H^k$ -norm by functions in (32).  $\square$

## 4.2 The Dirichlet Laplacian

Let  $\mathcal{L}$  be the linear partial differential expression

$$\mathcal{L} = -\Delta = -\sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}.$$

We say ‘‘expression’’ because we do not a priori specify whether  $\mathcal{L}$  acts on  $C^2$ -functions, or on functions in some Sobolev space, or even just as a distributional derivative; we will use the same symbol  $\mathcal{L}$  in all of these contexts. It is called the *negative Laplacian* (henceforth just ‘‘Laplacian’’), and we devote this section to constructing an appropriate realization of  $\mathcal{L}$  as a lower semibounded self-adjoint operator in  $L^2(\Omega)$ . For this we will need the *Green’s formulas*:

**Proposition 4.9** ([28, Theorem D.9]). *Suppose  $\Omega$  is bounded with  $C^2$ -boundary. Let  $\nu(x)$  be the outward unit normal vector at  $x \in \partial\Omega$  and let  $\sigma$  be the surface measure of  $\partial\Omega$ . For all  $h \in H^1(\Omega)$  and  $f, g \in H^2(\Omega)$ , we have*

$$\begin{aligned} \int_{\Omega} (-\Delta f)\bar{h} \, dx &= \int_{\Omega} \nabla f \cdot \overline{\nabla h} \, dx - \int_{\partial\Omega} \frac{\partial f}{\partial \nu} \bar{h} \, d\sigma, \\ \int_{\Omega} (-\Delta f)\bar{g} \, dx - \int_{\Omega} f \overline{(-\Delta g)} \, dx &= \int_{\partial\Omega} \left( f \frac{\partial \bar{g}}{\partial \nu} - \frac{\partial g}{\partial \nu} \bar{f} \right) d\sigma. \end{aligned}$$

Before we proceed, let us first recall the classical formulation of the boundary value problem for  $-\Delta$  on  $\Omega$ . For this purpose we introduce the sesquilinear form

$$\mathcal{D}(\mathfrak{t}) = H^1(\Omega) \quad \text{and} \quad \mathfrak{t}[f, g] = \int_{\Omega} \nabla f \cdot \overline{\nabla g} \, dx \quad \text{for} \quad f, g \in \mathcal{D}(\mathfrak{t}).$$

**Definition 4.10.** Suppose  $\Omega$  is bounded with  $C^1$ -boundary. Let  $f \in H^1(\Omega)$ ,  $g \in L^2(\Omega)$ ,  $h \in L^2(\partial\Omega)$ , and  $z \in \mathbb{C}$ . We say that  $f$  is a *weak solution* to the boundary value problem

$$\begin{cases} (-\Delta - z)f = g & \text{on } \Omega, \\ f = h & \text{on } \partial\Omega \end{cases} \quad (33)$$

if  $\mathfrak{t}[f, u] - z\langle f, u \rangle = \langle g, u \rangle$  for all  $u \in H_0^1(\Omega)$  and  $\text{Tr}(f) = h$ , where  $\text{Tr}$  is the trace operator associated to  $\Omega$ .

The classical approach to the Dirichlet eigenvalue problem (as used by for example Evans [10]) is in other words to take  $g = 0$  and  $h = 0$  in (33) and look for nontrivial weak solutions as  $z \in \mathbb{R}$  varies.

The notion of a weak solution to (33) with Dirichlet boundary conditions (i.e.  $h = 0$ ) can be equivalently formulated using the more modern notion of distributions: Observe that since  $C_0^\infty(\Omega)$  is dense in  $(H_0^1(\Omega), \|\cdot\|_{H^1(\Omega)})$ , the statement

$$\mathfrak{t}[f, u] - z\langle f, u \rangle = \langle g, u \rangle \quad \text{for all} \quad u \in H_0^1(\Omega)$$

is equivalent to

$$\mathfrak{t}[f, \varphi] - z\langle f, \varphi \rangle = \langle g, \varphi \rangle \quad \text{for all} \quad \varphi \in C_0^\infty(\Omega)$$

which by one of the Green's formulas (Proposition 4.9) is equivalent to

$$\int_{\Omega} f(-\Delta - z)\bar{\varphi} \, dx = \int_{\Omega} f\bar{\varphi} \, dx \quad \text{for all} \quad \varphi \in C_0^\infty(\Omega)$$

which is equivalent to  $(-\Delta - z)T_f = T_g$  in the sense of distributions. It follows by this and Theorem 4.5 that  $f \in H^1(\Omega)$  is a weak solution to

$$\begin{cases} (-\Delta - z)f = g & \text{on } \Omega, \\ f = 0 & \text{on } \partial\Omega \end{cases}$$

if and only if

$$\begin{cases} (-\Delta - z)T_f = T_g, \\ f \in H_0^1(\Omega). \end{cases}$$

This suggests that by restricting the distributional derivative operator  $-\Delta$  to an appropriate subspace of  $H_0^1(\Omega)$ , we can not only view  $-\Delta$  as an operator in  $L^2(\Omega)$ , but also encode the Dirichlet boundary condition into the operator itself. (A benefit of this is that we can drop the assumption of  $C^1$ -boundary since we are no longer using the trace operator explicitly.) This is essentially what we will do next, though in practice we will follow the approach of [28] and construct the Dirichlet Laplacian as a certain Friedrichs extension.

Given any  $f, g \in C_0^\infty(\Omega)$ , let  $\tilde{\Omega}$  be a bounded open set with  $C^2$ -boundary such that

$$(\text{supp } f) \cup (\text{supp } g) \subset \tilde{\Omega} \subset \Omega.$$

Since  $f, g$  are identically zero in a neighbourhood of  $\partial\tilde{\Omega}$ , the same is true for their normal derivatives  $\frac{\partial f}{\partial \nu}, \frac{\partial g}{\partial \nu}$ , and thus the Green's formulas gives

$$\begin{aligned} \int_{\tilde{\Omega}} (-\Delta f)\bar{g} \, dx &= \int_{\tilde{\Omega}} \nabla f \cdot \bar{\nabla} g \, dx, \\ \int_{\tilde{\Omega}} (-\Delta f)\bar{g} \, dx - \int_{\tilde{\Omega}} f\overline{(-\Delta g)} \, dx &= 0. \end{aligned}$$

Since  $f, g$  are identically zero also on  $\Omega \setminus \tilde{\Omega}$ , the above equations hold true when we replace  $\Omega$  with  $\tilde{\Omega}$ , and the resulting equations may be summarized as

$$\langle \mathcal{L}f, g \rangle = \langle f, \mathcal{L}g \rangle = \int_{\Omega} \nabla f \cdot \bar{\nabla} g \, dx.$$

In particular,

$$\langle \mathcal{L}f, f \rangle = \|\nabla f\|^2.$$

As a consequence we obtain a densely defined lower semibounded symmetric operator  $L_0$  in  $L^2(\Omega)$  by

$$\mathcal{D}(L_0) = C_0^\infty(\Omega) \quad \text{and} \quad L_0 = \mathcal{L}f \quad \text{for} \quad f \in \mathcal{D}(L_0).$$

We now proceed by constructing the Friedrichs extension of  $L_0$ . Following Section 2.10, we introduce a densely defined positive closable form  $\mathfrak{s}$  by

$$\mathcal{D}(\mathfrak{s}) = \mathcal{D}(L_0) \quad \text{and} \quad \mathfrak{s}[f, g] = \langle \mathcal{L}f, f \rangle \quad \text{for} \quad f, g \in \mathcal{D}(\mathfrak{s}),$$

and we aim to compute the closure of  $\mathfrak{s}$ . We observe that  $\mathfrak{s}$  is a restriction of  $\mathfrak{t}$ , but it turns out that the domain of the latter is too large to be the closure of the former. Instead, let us define

$$\mathfrak{t}_0 := \mathfrak{t} \upharpoonright H_0^1(\Omega) \times H_0^1(\Omega). \tag{34}$$

The quadratic form associated to  $\mathfrak{t}_0$  is given by

$$\mathfrak{t}_0[f] = \|\nabla f\|^2 \quad \text{for } f \in \mathcal{D}(\mathfrak{t}_0),$$

and since  $m = 0$  clearly is a lower bound of  $\mathfrak{t}_0$ , its form norm (which we recall is unique up to equivalence of forms) is given by

$$\|f\|_{\mathfrak{t}_0}^2 = \mathfrak{t}_0[f] + (1 - m)^2 \|f\|^2 = \|\nabla f\|^2 + \|f\|^2 = \|f\|_{H^1(\Omega)}^2,$$

where we have used (31). Since  $\mathfrak{s}$  is a restriction of  $\mathfrak{t}_0$ , the form norm of  $\mathfrak{s}$  is a restriction of the form norm of  $\mathfrak{t}_0$ . In other words, the normed space  $(\mathcal{D}(\mathfrak{s}), \|\cdot\|_{\mathfrak{s}}) = (C_0^\infty(\Omega), \|\cdot\|_{H^1(\Omega)})$  is a normed subspace of  $(\mathcal{D}(\mathfrak{t}_0), \|\cdot\|_{\mathfrak{t}_0}) = (H_0^1(\Omega), \|\cdot\|_{H^1(\Omega)})$ . Since  $H_0^1(\Omega)$  is by definition the closure of  $C_0^\infty(\Omega)$  with respect to the  $H^1(\Omega)$ -norm, we conclude that  $\bar{\mathfrak{s}} = \mathfrak{t}_0$ . Hence, by Theorem 2.13(iii), the Friedrichs extension of  $L_0$  can be constructed as

$$\mathcal{D}((L_0)_F) = \mathcal{D}((L_0)^*) \cap H_0^1(\Omega) \quad \text{and} \quad (L_0)_F = (L_0)^* \upharpoonright \mathcal{D}((L_0)_F).$$

To obtain a concrete description of the Friedrichs extension, we therefore require a concrete description of the adjoint of  $L_0$ . As the next proposition shows, this adjoint is the so-called *maximal operator*  $L_{\max}$ , which is defined as follows:  $f \in \mathcal{D}(L_{\max})$  if and only if  $\mathcal{L}T_f = T_g$  for some (necessarily unique)  $g \in L^2(\Omega)$ , in which case  $L_{\max}f := g$ .

**Proposition 4.11.**  $(L_0)^* = L_{\max}$ .

*Proof.* Let  $f \in L^2(\Omega)$ . By definition of the adjoint,  $f \in \mathcal{D}((L_0)^*)$  if and only if

$$\langle f, L_0\varphi \rangle = \langle g, \varphi \rangle \quad \text{for some } g \in L^2(\Omega) \quad \text{and all } \varphi \in \mathcal{D}(L_0),$$

and if this is the case, then  $(L_0)^*f = g$ . Since  $\mathcal{D}(L_0) = C_0^\infty(\Omega)$ , we have

$$\langle f, L_0\varphi \rangle = T_f(\overline{L_0\varphi}) = T_f(\mathcal{L}\bar{\varphi}) = (\mathcal{L}T_f)\bar{\varphi} \quad \text{and} \quad \langle g, \varphi \rangle = T_g\bar{\varphi}$$

for all  $\varphi \in C_0^\infty(\Omega)$ . Hence  $f \in \mathcal{D}((L_0)^*)$  if and only if

$$\mathcal{L}T_f = T_g \quad \text{for some } g \in L^2(\Omega),$$

and if this is the case, then  $(L_0)^*f = g$ . In other words,  $(L_0)^* = L_{\max}$  by the definition of the latter.  $\square$

**Definition 4.12.** The *Dirichlet Laplacian*  $-\Delta_D$  is the lower semibounded self-adjoint operator in  $L^2(\Omega)$  defined in any of the following equivalent ways:

- (i) as the Friedrichs extension of  $L_0$ ;
- (ii) as the unique self-adjoint operator corresponding to the densely defined positive closed form  $\mathfrak{t}_0$ ;
- (iii) as the restriction of  $L_{\max}$  to  $\mathcal{D}(L_{\max}) \cap H_0^1(\Omega)$ .

Note that unlike the definition of a weak solution, the definition of the Dirichlet Laplacian requires no additional assumptions on the open set  $\Omega$ . However, in order to gain a better understanding of  $-\Delta_D$  and especially its spectrum we must be willing to make at least some assumptions. To begin with, if we impose that  $\Omega$  is bounded (but without imposing any regularity whatsoever on the boundary of  $\Omega$ ) we obtain

**Proposition 4.13.** *Suppose  $\Omega$  is bounded. Then  $-\Delta_D$  has a purely discrete spectrum and its principal (lowest) eigenvalue is the largest constant  $c_\Omega$  for which Poincaré's inequality holds. In particular,  $-\Delta_D$  is a positive operator.*

*Proof.* As we recall, the form associated to  $-\Delta_D$  is  $t_0$ , so the form domain and form norm of  $-\Delta_D$  is  $(H_0^1(\Omega), \|\cdot\|_{H^1(\Omega)})$ . According to Proposition 4.4(i), this normed space is compactly embedded into its ambient Hilbert space, and hence  $-\Delta_D$  has a purely discrete spectrum by Proposition 2.6. Corollary 2.8 now says that the principal eigenvalue of  $-\Delta_D$  is given by

$$\lambda_1 = \inf_{\substack{f \in H_0^1(\Omega) \\ f \neq 0}} \frac{\|\nabla f\|^2}{\|f\|^2}.$$

The greatest  $c_\Omega$  for which Poincaré's inequality holds is exactly equal to the right-hand side, and this  $c_\Omega$  is positive by Proposition 4.4(ii). Since  $-\Delta_D$  has a purely discrete spectrum, its greatest lower bound is equal to the principal eigenvalue, which is  $c_\Omega$ , and thus  $-\Delta_D$  is positive.  $\square$

Due to this result we usually prefer to write  $\lambda_1(\Omega)$  instead of  $\mathfrak{m}(-\Delta_D)$  for the greatest lower bound when  $\Omega$  is bounded, since in this case the greatest lower bound and the principal eigenvalue are one and the same (as explained in Section 2.8). This notation also makes explicit the dependence on  $\Omega$ , which is convenient when we want to vary the domain, as we will do later.

If we in addition impose that  $\Omega$  has  $C^1$ -boundary, then Definition 4.12(iii) and Theorem 4.5 yield  $\mathcal{D}(-\Delta_D) = \mathcal{D}(L_{\max}) \cap \mathcal{N}(\text{Tr})$ , which we may interpret as saying that the domain of  $-\Delta_D$  consists of all functions  $f$  vanishing on the boundary of  $\Omega$  and such that  $-\Delta f$  makes sense. If the boundary of  $\Omega$  is sufficiently regular, then the domain and graph norm of  $-\Delta_D$  can in fact be determined explicitly:

**Proposition 4.14.** *Suppose  $\Omega$  is bounded with  $C^2$ -boundary. Then*

(i)  $\mathcal{D}(-\Delta_D) = H^2(\Omega) \cap H_0^1(\Omega);$

(ii) *the graph norm of  $-\Delta_D$  is equivalent to the  $H^2(\Omega)$ -norm on  $\mathcal{D}(-\Delta_D)$ .*

*Proof.*

- (i) Recall that  $\mathcal{D}(-\Delta_D) = \mathcal{D}(L_{\max}) \cap H_0^1(\Omega)$ . Obviously  $H^2(\Omega) \subset \mathcal{D}(L_{\max})$ , so  $H^2(\Omega) \cap H_0^1(\Omega) \subset \mathcal{D}(-\Delta_D)$ . By a so-called *regularity result* for the Dirichlet Laplacian, itself a special case of a regularity result for uniformly elliptic second-order linear partial differential operators, we have

$\mathcal{D}(-\Delta_D) \subset H^2(\Omega)$  [10, Section 6.3, Theorem 4]. (It is at this point that we use the assumption of  $C^2$ -boundary.) Therefore we also have the reverse inclusion  $\mathcal{D}(-\Delta_D) \subset H^2(\Omega) \cap H_0^1(\Omega)$ .

- (ii)  $-\Delta_D$  is self-adjoint and in particular closed, meaning  $(\mathcal{D}(-\Delta_D), \|\cdot\|_{-\Delta_D})$  is a Hilbert space.  $(H_0^1(\Omega), \|\cdot\|_{H^1(\Omega)})$  on the other hand is a Hilbert space by construction, and, since  $\|\cdot\|_{H^1(\Omega)} \leq \|\cdot\|_{H^2(\Omega)}$ , we see that  $(\mathcal{D}(-\Delta_D), \|\cdot\|_{H^2(\Omega)})$  is also a Hilbert space. To have equivalence between the two norms, it therefore suffices to show that one is stronger than the other [14, Corollary 4.6.3]. This is straightforward:

$$\begin{aligned} \|f\|_{-\Delta_D}^2 &= \|f\|^2 + \|-\Delta_D f\|^2 \\ &= \|f\|^2 + \sum_{i=1}^d \left\| -\frac{\partial^2 f}{\partial x_i^2} \right\|^2 \\ &\leq \|f\|_{H^2(\Omega)}^2. \end{aligned}$$

□

Finally, if the dimension is not too large, then  $-\Delta_D$  is guaranteed to act only on functions continuous up to the boundary:

**Proposition 4.15.** *Suppose  $d \leq 3$  and  $\Omega$  is bounded with  $C^2$ -boundary. Then  $\mathcal{D}(-\Delta_D) \subset C(\bar{\Omega})$ , and there exists a constant  $c > 0$  such that*

$$\sup_{x \in \bar{\Omega}} |f(x)| \leq c \|f\|_{-\Delta_D} \quad \text{for all } f \in \mathcal{D}(-\Delta_D).$$

*Proof.* By the previous proposition,  $\mathcal{D}(-\Delta_D) \subset H^2(\Omega)$ . Now use Proposition 4.6 along with the fact that the graph norm of  $-\Delta_D$  is equivalent to the  $H^2(\Omega)$ -norm, which again follows from the previous proposition. □

This implies in particular that the Dirichlet eigenvectors are continuous for  $d \leq 3$ , which in the case  $d = 2$  is vital for their physical interpretation as the standing waves of a vibrating drum shaped like  $\Omega$ .

### 4.3 The Green's function of the Dirichlet Laplacian

From now on we assume  $d \in \{2, 3\}$  and that  $\Omega$  is bounded, connected, and has  $C^\infty$ -boundary. Let

$$s(x, y) = \begin{cases} \frac{1}{\omega_2} \ln |x - y|^{-1} & \text{if } d = 2, \\ \frac{1}{\omega_3} |x - y|^{-1} & \text{if } d = 3, \end{cases}$$

where  $\omega_d$  is the surface measure of the unit sphere in  $\mathbb{R}^d$ . We use the shorthand  $s_y = s(\cdot, y)$ . We have

$$\frac{\partial}{\partial x_i} |x - y| = \frac{x_i - y_i}{|x - y|}$$

and thus

$$\frac{\partial}{\partial x_i} s_y = -\frac{1}{\omega_d} |x-y|^{-d} (x_i - y_i)$$

which gives

$$\nabla_x s_y = -\frac{1}{\omega_d} |x-y|^{-d} (x-y)$$

and

$$|\nabla_x s_y| = \frac{1}{\omega_d} |x-y|^{1-d}. \quad (35)$$

**Lemma 4.16.** *Let  $y \in \Omega$ . Then  $s_y \in L^2(\Omega)$ , but  $s_y \notin H^1(\Omega)$ .*

*Proof.* We may without loss of generality assume  $y = 0$ . Since  $s_0$  is smooth outside of the origin, it suffices to show that

$$\int_{B_\epsilon} |s_0|^2 dx < +\infty \quad \text{and} \quad \int_{B_\epsilon} |\nabla_x s_0|^2 dx = +\infty,$$

where  $B_\epsilon$ ,  $\epsilon > 0$  is the open ball of radius  $\epsilon$  centered at the origin, and  $\epsilon$  is small enough that  $B_\epsilon \subset \Omega$ . Let

$$f(r) = \begin{cases} \ln r^{-1} & \text{if } d = 2, \\ r^{-1} & \text{if } d = 3 \end{cases} \quad \text{for } r > 0.$$

By integrating in polar (hyperspherical) coordinates (see, e.g., [10, Appendix C, Theorem 4]),

$$\int_{B_\epsilon} |s_0|^2 dx = \frac{1}{\omega_d^2} \int_0^\epsilon r^{d-1} \int_{\partial B_1} f(r)^2 d\sigma dr = \frac{1}{\omega_d} \int_0^\epsilon f(r)^2 r^{d-1} dr.$$

Since  $f(r)r^{d-1}$  can be continuously extended to  $r = 0$ , we see that the rightmost integral is finite. Thus  $s_0 \in L^2(\Omega)$ . Next, by (35) and polar coordinates,

$$\int_{B_\epsilon} |\nabla_x s_y|^2 dx = \frac{1}{\omega_d^2} \int_0^\epsilon r^{d-1} \int_{\partial B_1} r^{2-2d} d\sigma dr = \frac{1}{\omega_d} \int_0^\epsilon r^{1-d} dr.$$

The rightmost integral is divergent, and hence  $s_0 \notin H^1(\Omega)$ .  $\square$

Let  $z \in \mathbb{C}$  and  $y \in \mathbb{R}^d$ . A *fundamental solution* of the linear partial differential expression  $-\Delta - z$  is a distribution  $E$  acting on  $\mathbb{R}^d$  such that  $(-\Delta - z)E = \delta_y$  in the sense of distributional derivatives. Since  $-\Delta - z$  has constant coefficients, such solutions always exist by the Malgrange-Ehrenpreis theorem [26]. Letting  $E' := E \upharpoonright C_0^\infty(\Omega)$ , we obtain a distribution  $E'$  on  $\Omega$  such that  $(-\Delta - z)E' = \delta_y$ . In what follows we will only be concerned with real  $z$  such that  $z < \lambda_1(\Omega)$ , so we will use  $\lambda$  instead of  $z$  to be consistent with our notation in Section 3. It turns out that in this case,  $E' = T_g$  for some unique  $g \in L^2(\Omega)$ . We shall now explain how to construct this  $g$ .

The following two definitions are equivalent to the one in [4, Section 1.1], but the reader should be aware of three things: Firstly, some authors define  $h^\lambda$

such that it differs in sign from ours, in which case one should take  $g_y^\lambda := s_y - h_y^\lambda$  instead of (37). Secondly, the name “relative Green’s function” does not seem to be standard, and often  $h_y^\lambda$  is not given any name at all; nevertheless, “relative Green’s function” is how the authors of [24] refer to  $h^\lambda$ , so we have chosen our terminology to agree with theirs. Thirdly,  $g^\lambda$  is sometimes defined in such a way that  $h^\lambda$  appears only implicitly in the definition and is not introduced in a stand-alone way, but as we will later see  $h^\lambda$  has an important role to play in this thesis and as such deserves its own name and notation.

**Definition 4.17.** Let  $\lambda < \lambda_1(\Omega)$ ,  $y \in \Omega$ , and let  $h_y^\lambda \in H^1(\Omega)$  be the unique weak solution to the boundary value problem

$$\begin{cases} (-\Delta - \lambda)h_y^\lambda = \lambda s_y & \text{on } \Omega, \\ h_y^\lambda = -s_y & \text{on } \partial\Omega. \end{cases} \quad (36)$$

The function  $h^\lambda(x, y) := h_y^\lambda(x)$  is called the *relative Green’s function of  $-\Delta - \lambda$  with respect to  $\Omega$* .

It is known that  $h^\lambda$  can be extended continuously to  $\bar{\Omega} \times \bar{\Omega}$  [4, Section 1.1].

**Definition 4.18.** Let  $\lambda < \lambda_1(\Omega)$ ,  $y \in \Omega$ , and let

$$g_y^\lambda := s_y + h_y^\lambda. \quad (37)$$

The function  $g^\lambda(x, y) := g_y^\lambda(x)$  is called the *Green’s function of  $-\Delta - \lambda$  with respect to  $\Omega$* .

It follows immediately from (37) that  $g^\lambda(x, \cdot) \in C(\bar{\Omega} \setminus \{x\}) \cap L^2(\Omega)$  and  $g^\lambda(\cdot, y) \in C(\bar{\Omega} \setminus \{y\}) \cap L^2(\Omega)$  for all  $x, y \in \Omega$ , and moreover  $g_y^\lambda = 0$  on  $\partial\Omega$  due to the boundary condition in (36). Note however that Proposition 4.15 implies  $g_y^\lambda \notin \mathcal{D}(-\Delta_D)$  due to the discontinuity at  $y$ .

We set out to find  $g \in L^2(\Omega)$  such that  $E' = T_g$ . As the next theorem shows,  $g_y^\lambda$  is exactly this  $g$ . (This implies that  $g_y^\lambda$  is not even in  $\mathcal{D}(L_{\max})$ , because if it were, then  $\delta_y$  would be of the form  $T_f$  for some  $f \in L^2(\Omega)$ , which is not true according to Lemma 4.3.) The result itself is stated as fact (but without being called a “theorem”) in [4, Section 1.1].

**Theorem 4.19.**  $(-\Delta - \lambda)T_{g_y^\lambda} = \delta_y$  in the sense of distributions.

As a consequence, we obtain that the Green’s functions are linearly independent:

**Corollary 4.20.**  $\{g_y^\lambda : y \in \Omega\}$  is a linearly independent set in  $L^2(\Omega)$ .

*Proof.* Any linear combination of the Green’s functions will, after applying the distributional derivative  $-\Delta - \lambda$  and using the theorem, result in a linear combination of some elements of  $\{\delta_x : x \in \Omega\}$ . If the former linear combination is equal to zero, then the latter is too, and then Lemma 4.2 implies that the coefficients must all be zero.  $\square$

For our purposes, the most important aspect of the Green's function is the fact that for each  $\lambda < \lambda_1(\Omega)$ , the resolvent  $(-\Delta_D - \lambda)^{-1}$  is an integral operator having the Green's function as integral kernel. Before giving a formal proof we shall first attempt to convince the reader of the validity of this statement. To this end, let  $f \in L^2(\Omega)$  and

$$h(x) := \int_{\Omega} g^\lambda(x, y) f(y) dy \quad \text{for all } x \in \bar{\Omega}.$$

The Cauchy-Schwarz inequality and (37) implies

$$\begin{aligned} |h(x)| &\leq \|g^\lambda(x, \cdot)\| \|f\| \\ &\leq \|h^\lambda(x, \cdot)\| \|f\| + \|s(x, \cdot)\| \|f\| \\ &\leq |\Omega| \|h^\lambda\|_\infty \|f\| + \|s_0\|_{L^2(\mathbb{R}^d)} \|f\| \end{aligned}$$

so  $h$  is bounded and hence in  $L^2(\Omega)$ . Letting  $\varphi \in C_0^\infty(\Omega)$  and  $\psi := (-\Delta - \lambda)\varphi$ , we compute

$$\begin{aligned} ((-\Delta - \lambda)T_h)\varphi &= T_h\psi \\ &= \int_{\Omega} h(x)\psi(x) dx \\ &= \int_{\Omega} \left( \int_{\Omega} g^\lambda(x, y) f(y) dy \right) \psi(x) dx \\ &= \int_{\Omega} f(y) \left( \int_{\Omega} g^\lambda(x, y) \psi(x) dx \right) dy \\ &= \int_{\Omega} f(y) T_{g_y^\lambda} \psi dy \\ &= \int_{\Omega} f(y) ((-\Delta - \lambda)T_{g_y^\lambda})\varphi dy \\ &= \int_{\Omega} f(y)\varphi(y) dy \\ &= T_f\varphi. \end{aligned}$$

where we have used the Fubini-Tonelli theorem and Theorem 4.19. It follows that  $h \in \mathcal{D}(L_{\max})$  and  $(L_{\max} - \lambda)h = f$  by definition of the maximal operator. If we also knew that  $h \in H_0^1(\Omega)$ , we could then conclude that  $h \in \mathcal{D}(-\Delta_D)$  and

$$((-\Delta_D - \lambda)^{-1}f)(x) = h(x) = \int_{\Omega} g^\lambda(x, y) f(y) dy \quad \text{for all } x \in \bar{\Omega}.$$

Instead of showing  $h \in H_0^1(\Omega)$ , however, we shall take a different approach.

**Proposition 4.21.** *Let  $\lambda < \lambda_1(\Omega)$ . Then  $(-\Delta_D - \lambda)^{-1}$  is an integral operator with kernel  $g^\lambda$ . In other words,*

$$((-\Delta_D - \lambda)^{-1}f)(x) = \int_{\Omega} g^\lambda(x, y) f(y) dy \quad \text{for all } f \in L^2(\Omega), x \in \bar{\Omega}.$$

*Proof.* Let us first note that Proposition 4.15 implies  $(-\Delta_D - \lambda)^{-1}f \in C(\overline{\Omega})$  for each  $f \in L^2(\Omega)$ , meaning  $((-\Delta_D - \lambda)^{-1}f)(x)$  is a well-defined complex number for each  $x \in \overline{\Omega}$ . Fix  $x \in \overline{\Omega}$  and let  $T_x : L^2(\Omega) \rightarrow \mathbb{C}$  be the linear functional defined by  $T_x f := ((-\Delta_D - \lambda)^{-1}f)(x)$ . Let  $f \in L^2(\Omega)$  and  $g := (-\Delta_D - \lambda)^{-1}f$ . Then  $(-\Delta_D)g = f + \lambda g$ . By the inequality  $(a + b)^2 \leq 2a^2 + 2b^2$  along with the boundedness of  $-\Delta_D - \lambda$  we get

$$\begin{aligned} \|g\|_{-\Delta_D}^2 &= \|g\|^2 + \|f + \lambda g\|^2 \\ &\leq \|g\|^2 + 2\|f\|^2 + 2\lambda^2 \|g\|^2 \\ &\leq C \|f\|^2 \end{aligned}$$

for some constant  $C > 0$ . According to Proposition 4.15, there also exists a constant  $c > 0$  such that

$$|T_x f| \leq c \|g\|_{-\Delta_D} \leq c\sqrt{C} \|f\|.$$

Therefore  $T_x$  is bounded. The Fréchet-Riesz representation theorem (see, e.g., [14, Theorem 6.2.4]) now furnishes a unique  $u_x \in L^2(\Omega)$  such that  $T_x f = \langle f, u_x \rangle$  for all  $f \in L^2(\Omega)$ . This provides us with our integral kernel, so we only have to show that  $\overline{u_x} = g^\lambda(x, \cdot)$  in the sense of  $L^2$ -functions.

Let  $\varphi \in C_0^\infty(\Omega)$  and  $\psi := (-\Delta_D - \lambda)^{-1}\varphi$ . This necessitates that  $\psi \in C^\infty(\overline{\Omega})$  by [10, Section 6.3, Theorem 6]; in particular,  $\psi$  is a classical (read: at least in  $C^2(\overline{\Omega})$ ) solution to the Dirichlet boundary value problem

$$\begin{cases} (-\Delta - \lambda)\psi = \varphi & \text{on } \Omega, \\ \psi = 0 & \text{on } \partial\Omega \end{cases}$$

It follows by the discussion in [4, Section 1.1] that  $\psi$  has the representation

$$\psi(x) = \int_{\Omega} g^\lambda(x, y)\varphi(y) dy \quad \text{for all } x \in \overline{\Omega},$$

while on the other hand

$$\psi(x) = ((-\Delta_D - \lambda)^{-1}\varphi)(x) = T_x \varphi = \langle \varphi, u_x \rangle = \int_{\Omega} \overline{u_x(y)}\varphi(y) dy,$$

and hence Lemma 4.1 implies that  $\overline{u_x} = g^\lambda(x, \cdot)$  in the sense of  $L^2$ -functions.  $\square$

**Proposition 4.22.** *Let  $\lambda < \lambda_1(\Omega)$  and  $x, y \in \Omega$ ,  $x \neq y$ . Then*

- (i)  $g^\lambda(x, y) > 0$ ;
- (ii)  $g^\lambda(x, y) = g^\lambda(y, x)$ ;
- (iii)  $\lambda \mapsto g^\lambda(x, y)$  is monotonically increasing on  $(-\infty, \lambda_1(\Omega))$ .

*Proof.*

- (i) This is stated in [24, Proposition 2.5(iii)].
- (ii) Since  $(-\Delta_D - \lambda)^{-1}$  is a self-adjoint integral operator, [31, Theorem 6.19] implies that  $(-\Delta_D - \lambda)^{-1}$  has  $(x, y) \mapsto \overline{g^\lambda(y, x)} = g^\lambda(y, x)$  as kernel, where the last equality follows from (i). This necessitates  $g^\lambda(x, y) = g^\lambda(y, x)$  a.e. on  $\Omega \times \Omega$ , which by continuity of the Green's function must therefore hold for all  $x, y \in \Omega, x \neq y$ .
- (iii) This is a consequence of (i) and [4, Section 1.2, Assertion (B)].

□

As an immediate consequence of this proposition and (37), we have

**Corollary 4.23.** *Let  $\lambda < \lambda_1(\Omega)$  and  $x, y \in \Omega$ . Then*

- (i)  $g^\lambda(x, y) \in \mathbb{R}$ ;
- (ii)  $g^\lambda(x, y) = g^\lambda(y, x)$ ;
- (iii)  $\lambda \mapsto g^\lambda(x, y)$  is monotonically increasing on  $(-\infty, \lambda_1(\Omega))$ .

The following two identities will play an important role in the next section.

**Proposition 4.24.** *Let  $\lambda, \mu < \lambda_1(\Omega)$  and  $x, y \in \Omega$ . Then*

- (i)  $g_y^\mu = (-\Delta_D - \lambda)(-\Delta_D - \mu)^{-1}g_y^\lambda$ ;
- (ii)  $h^\mu(x, y) - h^\lambda(x, y) = (\mu - \lambda)\langle g_x^\mu, g_y^\lambda \rangle$ .

*Proof.* By writing  $-\Delta_D - \lambda = (-\Delta_D - \mu) + (\mu - \lambda)$ , we see that

$$(-\Delta_D - \lambda)(-\Delta_D - \mu)^{-1} = I + (\mu - \lambda)(-\Delta_D - \mu)^{-1}.$$

Hence (i) is equivalent to

$$g_y^\mu - g_y^\lambda = (-\Delta_D - \mu)^{-1}((\mu - \lambda)g_y^\lambda).$$

On the other hand,  $G := (-\Delta_D - \mu)^{-1}((\mu - \lambda)g_y^\lambda)$  is the unique weak solution to the boundary value problem

$$\begin{cases} (-\Delta - \mu)G = (\mu - \lambda)g_y^\lambda & \text{on } \Omega, \\ G = 0 & \text{on } \partial\Omega. \end{cases}$$

It therefore suffices to show that  $G' := g_y^\mu - g_y^\lambda$  solves this problem. The boundary condition is clearly correct, as  $g_y^\mu = g_y^\lambda = 0$  on  $\partial\Omega$ . By (37),  $G' = h_y^\mu - h_y^\lambda$ . By (36),  $(-\Delta - \mu)h_y^\mu = \mu s_y$ . As for the other relative Green's function, we use the same trick as above and write

$$(-\Delta - \mu)h_y^\lambda = ((-\Delta - \lambda) + (\lambda - \mu))h_y^\lambda = \lambda s_y + (\lambda - \mu)h_y^\lambda.$$

Hence

$$(-\Delta - \mu)G' = \mu s_y - \lambda s_y + (\mu - \lambda)h_y^\lambda = (\mu - \lambda)(h_y^\lambda - s_y) = (\mu - \lambda)g_y^\lambda$$

where the last equality is by (37). This proves (i). As for (ii), we use Proposition 4.21 to evaluate

$$G(x) = (\mu - \lambda)((-\Delta_D - \mu)^{-1}g_y^\lambda)(x) = (\mu - \lambda)\langle g_y^\lambda, g_x^\mu \rangle = (\mu - \lambda)\langle g_x^\mu, g_y^\lambda \rangle$$

where we in the last equality used that the Green's functions are real-valued. As for the left-hand side,  $G(x) = h_y^\mu(x) - h_y^\lambda(x) = h^\mu(x, y) - h^\lambda(x, y)$ . This completes the proof.  $\square$

#### 4.4 Construction of the Hamiltonian

In what follows, let  $X$  be a fixed, finite and nonempty subset of  $\Omega$ . We know by Proposition 4.15 that  $f(x)$  is a well-defined complex number for all  $f \in \mathcal{D}(-\Delta_D)$  and  $x \in \Omega$ , so we can define an operator  $H$  by restricting  $-\Delta_D$  to the domain

$$\mathcal{D}(H) = \{f \in \mathcal{D}(-\Delta_D) : f(x) = 0 \text{ for all } x \in X\}.$$

For any  $\lambda \in \mathbb{C}$ , we write  $\mathcal{N}_\lambda := \mathcal{N}(H^* - \lambda)$ .

**Proposition 4.25.**  *$H$  is a densely defined lower semibounded closed operator with Friedrichs extension  $-\Delta_D$ .*

*Proof.* Symmetry and lower semiboundedness follows immediately from being a restriction of the self-adjoint, lower semibounded operator  $-\Delta_D$ .

As for the density, note that  $\mathcal{D}(H)$  contains the set (32), so by taking  $k = 0$  in Lemma 4.8 we find that  $\mathcal{D}(H)$  is dense in  $H_0^0(\Omega)$ . Since the latter is by definition the closure of  $C_0^\infty(\Omega)$  in  $L^2(\Omega)$  and thus equal to  $L^2(\Omega)$  by Lemma 4.1, we obtain the density of  $\mathcal{D}(H)$  in  $L^2(\Omega)$ .

To show that  $H$  is closed, we must show that  $(\mathcal{D}(H), \|\cdot\|_H)$  is a Banach space. Let  $\{f_n\}$  be a Cauchy sequence in  $(\mathcal{D}(H), \|\cdot\|_H)$ . Since the graph norm of  $H$  is a restriction of the graph norm of  $-\Delta_D$ , and  $(\mathcal{D}(-\Delta_D), \|\cdot\|_{-\Delta_D})$  is a Banach space, we see that  $f_n$  converges in  $\|\cdot\|_{-\Delta_D}$ -norm to some  $f \in \mathcal{D}(-\Delta_D)$ . Let  $x \in X$ . Then, by Proposition 4.15, there exists  $c > 0$  such that

$$|f(x)| = |f(x) - f_n(x)| \leq c \|f - f_n\|_{-\Delta_D} \quad \text{for all } n \in \mathbb{N}.$$

Letting  $n \rightarrow \infty$  gives  $f(x) = 0$ , and since  $x \in X$  was arbitrary,  $f \in \mathcal{D}(H)$ . Therefore  $\{f_n\}$  has a  $\|\cdot\|_H$ -limit in  $\mathcal{D}(H)$ , and  $H$  is a closed operator.

In view of Lemma 2.14, Definition 4.12, and (34), we have  $H_F = -\Delta_D$  if and only if  $\mathcal{D}(H)$  is dense in  $(H_0^1(\Omega), \|\cdot\|_{H^1(\Omega)})$ . Let  $k = 1$ . Since  $\mathcal{D}(H)$  contains the set (32), we see that in the case  $d = 3$  the inequality  $2k + 1 \leq d$  holds and thus the density follows by Lemma 4.8. This argument does not work when  $d = 2$ , so for the general case we instead refer to [24, Section 3] where it is stated that “[ $-\Delta_D$ ], obviously a self-adjoint extension of [ $H$ ], is precisely the Friedrichs extension of [ $H$ ].”  $\square$

**Theorem 4.26.** *Let  $\lambda < \lambda_1(\Omega)$ . Then  $\{g_x^\lambda : x \in X\}$  is a basis of  $\mathcal{N}_\lambda$ .*

*Proof.*  $\lambda < \lambda_1(\Omega)$  implies  $\lambda \in \rho(-\Delta_D)$ , so  $-\Delta_D - \lambda$  is a bijection of  $\mathcal{D}(-\Delta_D)$  onto  $L^2(\Omega)$ . Moreover,  $H - \lambda$  is a restriction of  $-\Delta_D - \lambda$ , and therefore a bijection of  $\mathcal{D}(H)$  onto  $\mathcal{R}(H - \lambda)$  whose inverse is a restriction of  $(-\Delta_D - \lambda)^{-1}$ . Hence  $(-\Delta_D - \lambda)^{-1}$  maps  $\mathcal{R}(H - \lambda)$  bijectively onto  $\mathcal{D}(H)$ . This implies

$$\begin{aligned} \mathcal{R}(H - \lambda) &= \{f \in L^2(\Omega) : (-\Delta_D - \lambda)^{-1}f \in \mathcal{D}(H)\} \\ &= \{f \in L^2(\Omega) : ((-\Delta_D - \lambda)^{-1}f)(x) = 0 \text{ for all } x \in X\} \\ &= \{f \in L^2(\Omega) : \langle f, g_x^\lambda \rangle = 0 \text{ for all } x \in X\} \\ &= (\text{span}\{g_x^\lambda : x \in X\})^\perp \end{aligned}$$

where we have used Proposition 4.21 in the third equality. Taking orthogonal complements of both sides and using the fact that finite-dimensional subspaces are closed yields

$$\text{span}\{g_x^\lambda : x \in X\} = \mathcal{R}(H - \lambda)^\perp = \mathcal{N}(H^* - \lambda) = \mathcal{N}_\lambda.$$

The linear independence of the Green's functions was shown in Corollary 4.20, and since they span  $\mathcal{N}_\lambda$  they are therefore a basis.  $\square$

Henceforth, let  $m = |X|$  denote the cardinality of  $X$ .

**Corollary 4.27.** *The defect indices of  $H$  are  $(m, m)$ .*

*Proof.* The above theorem implies  $\dim(\mathcal{N}_\lambda) = m$ . Now use Proposition 2.10.  $\square$

Let us now assume that we have chosen some fixed but otherwise arbitrary enumeration  $\{x_1, x_2, \dots, x_m\} = X$ . For each  $\lambda < \lambda_1(\Omega)$ , define a corresponding ordered basis  $\mathbb{G}_\lambda$  of  $\mathcal{N}_\lambda$  by ordering the Green's functions in the obvious way:

$$\mathbb{G}_\lambda := (g_1^\lambda, \dots, g_m^\lambda) := (g_{x_1}^\lambda, \dots, g_{x_m}^\lambda).$$

Let  $\mathbb{G} := \{\mathbb{G}_\lambda : \lambda < \lambda_1(\Omega)\}$  and recall the terminology of Section 3.5.

**Proposition 4.28.**  *$\mathbb{G}$  is a gamma family for  $(H, -\Delta_D)$  on  $(-\infty, \lambda_1(\Omega))$ .*

*Proof.* Let  $\lambda, \mu < \lambda_1(\Omega)$ . Since  $-\Delta_D$  is a self-adjoint extension of the densely defined symmetric operator  $H$  we can construct a designated boundary triplet  $(H^*, \Gamma_0^\lambda, \Gamma_1^\lambda)$  for  $H^*$  as in Section 3.2. This boundary triplet furnishes an associated gamma field  $\gamma_\lambda : \rho(-\Delta_D) \rightarrow \mathcal{B}(\mathcal{N}_\lambda, L^2(\Omega))$  which Proposition 3.13(i) asserts has the form

$$\gamma_\lambda(z) = (-\Delta_D - \lambda)(-\Delta_D - z)^{-1} \quad \text{for all } z \in \rho(-\Delta_D).$$

Proposition 4.24(i) is then equivalent to the statement

$$g_y^\lambda = \gamma_\lambda(\mu)g_y^\mu \quad \text{for all } \lambda, \mu < \lambda_1(\Omega), y \in \Omega$$

and this statement implies  $\mathbb{G}_\mu = \gamma_\lambda(\mu)\mathbb{G}_\lambda$  in the sense of (20). In other words,  $\mathbb{G}_\mu$  and  $\mathbb{G}_\lambda$  are gamma compatible.  $\square$

We next define two real symmetric  $m \times m$  matrices: Let  $\mathbf{G}(\lambda) := (\langle g_i^\lambda, g_j^\lambda \rangle)_{ij}$  and let  $\mathbf{H}(\lambda)$  be the matrix with entries

$$\mathbf{H}(\lambda)_{ij} = \begin{cases} h^\lambda(x_i, x_i) & \text{if } i = j, \\ g^\lambda(x_i, x_j) & \text{if } i \neq j. \end{cases}$$

Recall the terminology of Section 3.6.

**Proposition 4.29.**  $\mathbf{H}(\lambda)$  is a Weyl primitive for  $\mathbb{G}$ .

*Proof.*  $\mathbf{H}(\lambda)$  is real and symmetric and therefore Hermitian. We must show that  $\mathbf{M}(\mu, \lambda) = \mathbf{H}(\mu) - \mathbf{H}(\lambda)$  for all  $\lambda, \mu < \lambda_1(\Omega)$ . By Lemma 3.31 and Proposition 4.24(ii) we have, for all  $i, j = 1, \dots, m$ ,

$$\mathbf{M}(\mu, \lambda)_{ij} = \mathbf{e}_i^T \mathbf{M}(\mu, \lambda) \mathbf{e}_j = (\mu - \lambda) \langle g_j^\mu, g_i^\lambda \rangle = h^\mu(x_j, x_i) - h^\lambda(x_j, x_i)$$

where  $\mathbf{e}_i := (\delta_{1i}, \delta_{2i}, \dots, \delta_{mi})^T$ . This takes care of the diagonal. For the non-diagonal elements we only have to note that (37) implies  $h^\mu(x, y) - h^\lambda(x, y) = g^\mu(x, y) - g^\lambda(x, y)$  for all  $x, y \in \Omega$ ,  $x \neq y$  and use the symmetry of  $g^\lambda$ .  $\square$

In summary, we have proved

**Theorem 4.30.**  $(H, \mathbb{G}, \mathbf{H})$  is an admissible operator.

**Corollary 4.31.**  $\lambda \mapsto \mathbf{H}(\lambda)$  is strictly increasing, analytic with derivative  $\mathbf{H}'(\lambda) = \mathbf{G}(\lambda)$ , and

$$\lim_{\lambda \rightarrow -\infty} \mathbf{u}^H \mathbf{H}(\lambda) \mathbf{u} = -\infty \quad \text{for all } \mathbf{u} \in \mathbb{C} \setminus \{0\}.$$

*Proof.* This is Proposition 3.41 applied to the particular Weyl primitive  $\mathbf{H}$ . The last assertion holds because  $\mathbf{H}$  is a Weyl primitive for  $\mathbb{G}$ , which is a gamma family for  $(H, -\Delta_D)$ , and  $-\Delta_D$  is the Friedrichs extension of  $H$  by Proposition 4.25.  $\square$

It might seem strange to use  $\mathbf{H}(\lambda)$  as Weyl primitive when the matrix  $(h^\lambda(x_i, x_j))_{ij}$  would also work. However, the former Weyl primitive makes possible a physical interpretation of the self-adjoint extensions of  $H$  generated by Theorem 3.43(i) in the special case that  $\mathbf{B}$  is diagonal. For this, let us use the shorthand

$$H_\alpha = H_{\text{diag}(\alpha_1, \dots, \alpha_m)} \quad \text{for } \alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{R}^m.$$

**Proposition 4.32.** Let  $u \in \mathcal{D}(H_\alpha)$ ,  $\alpha \in \mathbb{R}^m$ . Then there exist  $c_i \in \mathbb{C}$  such that for each  $i = 1, 2, \dots, m$ ,

$$u(x) = (s(x, x_i) + \alpha_i) c_i + o(1) \quad \text{as } x \rightarrow x_i. \quad (38)$$

*Proof.* Let  $\lambda < \lambda_1(\Omega)$  and  $\mathbf{C} := \mathbf{B} - \mathbf{H}(\lambda)$ . Recall that  $H$  is closed by Proposition 4.25. By Theorem 3.43(i) there exist  $f \in \mathcal{D}(H)$ ,  $\mathbf{u} \in \mathbb{C}^m$  such that

$$u = f + (-\Delta_D - \lambda)\mathbf{C}_\lambda \mathbf{u}_\lambda + \mathbf{u}_\lambda.$$

The first two terms are continuous functions on  $\Omega$  by Proposition 4.15. Moreover,  $f(x_i) = 0$ . Thus

$$u(x) = ((-\Delta_D - \lambda)\mathbf{C}_\lambda \mathbf{u}_\lambda)(x_i) + \mathbf{u}_\lambda(x) + o(1) \quad \text{as } x \rightarrow x_i.$$

Let  $\mathbf{e}_i = (\delta_{1i}, \dots, \delta_{mi})^T$ . We compute

$$\begin{aligned} ((-\Delta_D - \lambda)\mathbf{C}_\lambda \mathbf{u}_\lambda)(x_i) &= \langle \mathbf{C}_\lambda \mathbf{u}_\lambda, g_{x_i}^\lambda \rangle \\ &= \langle \mathbf{C}_\lambda \mathbf{u}_\lambda, (\mathbf{e}_i)_\lambda \rangle \\ &= \mathbf{e}_i^T \mathbf{C} \mathbf{u} \\ &= \sum_j \mathbf{C}_{ij} \mathbf{u}_j \\ &= \alpha_i \mathbf{u}_i - \sum_j \mathbf{H}(\lambda)_{ij} \mathbf{u}_j. \end{aligned}$$

Next we consider the term  $\mathbf{u}_\lambda(x)$ . As  $x \mapsto h^\lambda(x, x_i)$  is continuous on  $\Omega$ , we have

$$g_i^\lambda(x) = s(x, x_i) + h^\lambda(x, x_i) = s(x, x_i) + \mathbf{H}(\lambda)_{ii} + o(1) \quad \text{as } x \rightarrow x_i.$$

Moreover, as  $g_j^\lambda(x) = g^\lambda(x, x_j)$  is continuous on  $\Omega \setminus \{x_j\}$ , we have for all  $j \neq i$ ,

$$g_j^\lambda(x) = \mathbf{H}(\lambda)_{ij} + o(1) \quad \text{as } x \rightarrow x_i.$$

Thus

$$\begin{aligned} \mathbf{u}_\lambda(x) &= \sum_j \mathbf{u}_j g_j^\lambda(x) \\ &= s(x, x_i) \mathbf{u}_i + \sum_j \mathbf{H}(\lambda)_{ij} \mathbf{u}_j + o(1) \quad \text{as } x \rightarrow x_i. \end{aligned}$$

In summary,

$$u(x) = (s(x, x_i) + \alpha_i) \mathbf{u}_i + o(1) \quad \text{as } x \rightarrow x_i,$$

so the assertion holds with  $c_i = \mathbf{u}_i$ ,  $i = 1, 2, \dots, m$ .  $\square$

A careful read of [8, Section III] makes clear that in the case  $d = 3$ , our extension  $H_\alpha$  is exactly equal to their extension  $H^{(\alpha_i \delta_{ij})_{ij} (\delta_{ij})_{ij}}$ . Since the latter extensions constitute what the authors of [8] call “the most general extension[s] of the local kind,” or, in their introduction, “point interaction operators in [a] bounded domain,” we will borrow some of this terminology and say:

**Definition 4.33.**  $H_\alpha$  is called a *point-interaction Hamiltonian* in  $\Omega$ .

## 4.5 Spectral properties of the Hamiltonian

**Proposition 4.34.**  $H_\alpha$  has a purely discrete spectrum for all  $\alpha \in \mathbb{R}^m$ .

*Proof.* Recall that to have a purely discrete spectrum means to have an empty essential spectrum.  $H$  is a closed symmetric operator in a complex Hilbert space with equal finite defect indices, so by [31, Theorem 8.18] all self-adjoint extensions of  $H$  have the same essential spectrum. Since  $-\Delta_D$  is a self-adjoint extension of  $H$ , and  $-\Delta_D$  has a purely discrete spectrum by Proposition 4.13, we conclude that  $H_\alpha$  also has a purely discrete spectrum.  $\square$

In view of the above proposition, we will switch to the notation

$$\lambda_1(\Omega, X, \alpha) = \mathfrak{m}(H_\alpha) \quad \text{for } \alpha \in \mathbb{R}^m.$$

This reflects the fact that, similarly to the Dirichlet Laplacian, the greatest lower bound of  $H_\alpha$  is equal to the principal eigenvalue. Including the explicit dependence on  $\Omega$  and  $X$  will also be convenient when we later let  $\Omega$  and  $X$  vary.

**Proposition 4.35.**  $\lambda_1(\Omega, X, \alpha) < \lambda_1(\Omega)$  for all  $\alpha \in \mathbb{R}^m$ .

*Proof.* Let  $f$  be an eigenfunction of  $-\Delta_D$  corresponding to the smallest eigenvalue  $\lambda_1(\Omega)$ . As is explained in [18, Section 1.3.3], we can choose  $f$  nonnegative on  $\Omega$ . Since the Green's function  $g^\lambda$  is positive on  $\Omega \times \Omega$  and  $f \neq 0$ , we have  $(f, g_x^\lambda) > 0$  for any  $x \in X$ . Now the assertion follows from Proposition 3.4.  $\square$

Fix  $\alpha \in \mathbb{R}^m$ . According to Theorem 3.44, the value and eigenspace of  $\lambda_1(\Omega, X, \alpha)$  is controlled by the function

$$F(\alpha, \lambda) := \lambda_{\max}(\mathbf{H}(\lambda) - \text{diag}(\alpha)) \quad \text{for } \lambda < \lambda_1(\Omega). \quad (39)$$

More specifically, we have  $\lambda = \lambda_1(\Omega, X, \alpha)$  if and only if  $F(\alpha, \lambda) = 0$ , and then

$$\mathcal{N}(H_\alpha - \lambda) = \{\mathbf{u}_\lambda : \mathbf{u} \in \mathcal{N}(\mathbf{H}(\lambda) - \text{diag}(\alpha))\} \quad (40)$$

where

$$\mathbf{u}_\lambda := \sum_{i=1}^m \mathbf{u}_i g_i^\lambda.$$

**Proposition 4.36.**  $F(\alpha, \lambda)$  is a simple eigenvalue of  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$ , and the corresponding eigenvector is positive, i.e., each entry is positive.

*Proof.* Choose  $\tau \in \mathbb{R}$  such that

$$\min_{1 \leq i \leq m} (h^\lambda(x_i, x_i) - \alpha_i) + \tau > 0.$$

Then all the diagonal entries of  $\mathbf{H}(\lambda) - \text{diag}(\alpha) + \tau \mathbf{I}$  are positive. Since Proposition 4.22(i) furthermore implies that all the off-diagonal entries also are positive,  $\mathbf{H}(\lambda) - \text{diag}(\alpha) + \tau \mathbf{I}$  is a positive matrix (i.e., all entries are positive). It follows by the Perron-Frobenius theorem (see, e.g., [7, Theorem 2.1.4]) that the largest

eigenvalue of  $\mathbf{H}(\lambda) - \text{diag}(\alpha) + \tau\mathbf{I}$  is simple and the corresponding eigenvector can be chosen to have all entries positive. Then, since adding the factor  $\tau\mathbf{I}$  to  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$  only translates the spectrum of the latter and moreover does not affect the eigenvectors, the assertion follows.  $\square$

**Lemma 4.37.** *Let  $\lambda(t)$ ,  $\mathbf{q}(t)$ , and  $\mathbf{A}(t)$  be differentiable families of scalars, unit vectors, and symmetric matrices, respectively. If  $\mathbf{A}(t)\mathbf{q}(t) = \lambda(t)\mathbf{q}(t)$ , then  $\lambda'(t) = \mathbf{q}(t)^H \mathbf{A}'(t)\mathbf{q}(t)$ .*

*Proof.* We compute

$$\begin{aligned} \lambda'(t) - \mathbf{q}(t)^H \mathbf{A}'(t)\mathbf{q}(t) &= \mathbf{q}'(t)^H \mathbf{A}(t)\mathbf{q}(t) + \mathbf{q}(t)^H \mathbf{A}(t)\mathbf{q}'(t) \\ &= \lambda(t)\mathbf{q}'(t)^H \mathbf{q}(t) + \lambda(t)\mathbf{q}(t)^H \mathbf{q}'(t) \\ &= \lambda(t) \frac{d}{dt} (\mathbf{q}(t)^H \mathbf{q}(t)) \\ &= \lambda(t) \frac{d}{dt} (1) \\ &= 0. \end{aligned}$$

$\square$

**Proposition 4.38.**  *$F(\alpha, \lambda)$  is analytic separately in each argument, and*

$$\frac{\partial F}{\partial \lambda} = \|\mathbf{u}_\lambda\|^2, \quad \frac{\partial F}{\partial \alpha_i} = -|\mathbf{u}_i|^2 \quad \text{for all } i = 1, 2, \dots, m,$$

where  $\mathbf{u}$  is the normalized eigenvector corresponding to  $F(\alpha, \lambda)$ . In particular,  $F(\alpha, \lambda)$  is strictly increasing in  $\lambda$  and strictly decreasing in each  $\alpha_i$ .

*Proof.* Since  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$  is an analytic family of Hermitian matrices, both in  $\lambda$  (by Corollary 4.31) and in each  $\alpha_i$  (obvious), we have by [22, Section II, Theorem 6.1] that  $F(\alpha, \lambda)$  is analytic separately in each argument. Moreover, by [22, Section II§6.2], we can choose a family of orthonormal eigenbases such that each eigenvector is analytic in any individual argument of our choice. In particular, the normalized maximal eigenvector  $\mathbf{u} = \mathbf{u}(\alpha, \lambda)$  can be chosen analytic with respect to any one of the individual arguments  $\lambda, \alpha_1, \dots, \alpha_m$ . Now

$$\frac{\partial}{\partial \lambda} (\mathbf{H}(\lambda) - \text{diag}(\alpha)) = \mathbf{G}(\lambda), \quad \frac{\partial}{\partial \alpha_i} (\mathbf{H}(\lambda) - \text{diag}(\alpha)) = -\text{diag}(\delta_{1i}, \dots, \delta_{mi}),$$

where the first partial derivative follows from by Corollary 4.31 and the second is obvious. Hence, by Lemma 4.37,

$$\frac{\partial F}{\partial \lambda} = \mathbf{u}^H \mathbf{G}(\lambda)\mathbf{u} = \|\mathbf{u}_\lambda\|^2, \quad \frac{\partial F}{\partial \alpha_i} = -\mathbf{u}^H \text{diag}(\delta_{1i}, \dots, \delta_{mi})\mathbf{u} = -|\mathbf{u}_i|^2.$$

$\square$

**Theorem 4.39.** *Let  $\lambda := \lambda_1(\Omega, X, \alpha)$ . Then  $\lambda$  is a simple eigenvalue of  $H_\alpha$  with corresponding eigenfunction  $\mathbf{u}_\lambda$ , where  $\mathbf{u}$  is the unique positive solution to*

$$\mathbf{H}(\lambda)\mathbf{u} = \text{diag}(\alpha)\mathbf{u}.$$

*Furthermore, each map  $\alpha_i \mapsto \lambda_1(\Omega, X, \alpha)$  is analytic with derivative*

$$\frac{\partial}{\partial \alpha_i} \lambda_1(\Omega, X, \alpha) = \frac{|\mathbf{u}_i|^2}{\|\mathbf{u}_{\lambda_1}\|^2}$$

*and hence strictly increasing.*

*Proof.* The first few assertions follow from Proposition 4.36 and (40). Since  $\lambda_1(\alpha_i) := \lambda_1(\Omega, X, \alpha)$  (all other  $\alpha_j$  held constant) is the unique solution of  $F(\alpha, \lambda) = 0$ , we have by the analytic implicit function theorem in one variable that  $\lambda_1(\alpha_i)$  is analytic, and, assuming  $\mathbf{u}$  is normalized,

$$\frac{\partial}{\partial \alpha_i} \lambda_1(\alpha_i) = - \left( \frac{\partial F}{\partial \lambda} \right)^{-1} \frac{\partial F}{\partial \alpha_i} = \frac{|\mathbf{u}_i|^2}{\|\mathbf{u}_{\lambda_1}\|^2},$$

where we have used Proposition 4.38. If  $\mathbf{u}$  is not normalized, then we may first multiply  $\mathbf{u}$  by a constant so that it becomes normalized, but note that this does not change the above derivative, as the constant is cancelled out in the fraction.  $\square$

**Proposition 4.40.** *With notation as in Theorem 4.39, let  $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_m)$ . The eigenfunction  $\mathbf{u}_\lambda$  has the alternative representation  $\mathbf{u}_\lambda = f + \mathbf{u}_0$ , where*

$$\begin{aligned} \mathbf{u}_0 &:= \sum_i \mathbf{u}_i g_i^0 \in \mathcal{N}_0, \\ f &:= \sum_i \mathbf{u}_i (h_{x_i}^\lambda - h_{x_i}^0) \in H_0^1(\Omega) \cap C(\bar{\Omega}). \end{aligned}$$

*If in addition  $\lambda \geq 0$  (resp.  $\lambda \leq 0$ ), then  $f \geq 0$  ( $f \leq 0$ ).*

*Proof.* Taking  $\lambda = 0$  in Theorem 3.43(ii), we see that  $\mathbf{u}_\lambda \in \mathcal{D}(H_\alpha) \subset \mathcal{D}[H_\alpha] = \mathcal{D}[-\Delta_D] \dot{+} \mathcal{N}_0 = H_0^1(\Omega) \dot{+} \text{span}\{g_i^0 : i = 1, \dots, m\}$ . Thus there exist unique  $f \in H_0^1(\Omega)$  and  $\mathbf{v} \in \mathbb{C}^m$  such that  $\mathbf{u}_\lambda = f + \mathbf{v}_0$ . Since  $\mathbf{u}_\lambda$  and  $\mathbf{v}_0$  are continuous except on  $X$ , we see that  $f = \mathbf{u}_\lambda - \mathbf{v}_0$  is also continuous except possibly at some points in  $X$ . In view of (37), we have

$$\mathbf{u}_\lambda(x) = \mathbf{u}_i s_{x_i}(x) + C_i + o(1) \quad \text{as } x \rightarrow x_i$$

for some constant  $C_i \in \mathbb{R}$ , and similarly

$$\mathbf{v}_0(x) = \mathbf{v}_i s_{x_i}(x) + D_i + o(1) \quad \text{as } x \rightarrow x_i$$

for some constant  $D_i \in \mathbb{R}$ . Hence

$$f(x) = (\mathbf{u}_i - \mathbf{v}_i) s_{x_i}(x) + C_i - D_i + o(1) \quad \text{as } x \rightarrow x_i.$$

We have  $f \in H_0^1(\Omega)$ , but also  $s_{x_i} \notin H^1(\Omega)$  by Lemma 4.16, so it is necessary that  $\mathbf{u}_i = \mathbf{v}_i$  for all  $i$ . Therefore  $\mathbf{u}_\lambda = f + \mathbf{u}_0$ , and

$$f = \mathbf{u}_\lambda - \mathbf{u}_0 = \sum \mathbf{u}_i(g_i^\lambda - g_i^0) = \sum \mathbf{u}_i(h_{x_i}^\lambda - h_{x_i}^0).$$

The last assertion follows from this expression for  $f$  along with the fact that  $\lambda \mapsto h_{x_i}^\lambda(y)$  is monotonously increasing for each  $y \in \Omega$  by Corollary 4.23.  $\square$

With  $\Omega$  and  $X = \{x_1, \dots, x_m\}$  as before, suppose now that we add a new distinct point  $x_{m+1} \in \Omega$  to our set  $X$ , yielding a larger set  $X' = X \cup \{x_{m+1}\}$ . We may then assign a new interaction strength parameter at  $x_{m+1}$  and correspondingly use a larger tuple  $\alpha' = (\alpha, \alpha_{m+1}) \in \mathbb{R}^{m+1}$  of parameters. The next theorem generalizes Proposition 4.35.

**Theorem 4.41.**  $\lambda_1(\Omega, X', \alpha') < \lambda_1(\Omega, X, \alpha)$  for all  $\alpha' = (\alpha, \alpha_{m+1}) \in \mathbb{R}^{m+1}$ .

*Proof.* Let  $\mathbf{H}(\lambda)$  denote the Weyl primitive before adding the point, and let  $\mathbf{H}_1(\lambda)$  denote the Weyl primitive after adding the point. Then  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$  is the leading principal submatrix of order  $m$  of the  $(m+1) \times (m+1)$  Hermitian matrix  $\mathbf{H}_1(\lambda) - \text{diag}(\alpha')$ . Therefore, by the Cauchy interlace theorem (see, e.g., [20, Theorem 1]),

$$\lambda_{\max}(\mathbf{H}(\lambda) - \text{diag}(\alpha)) \leq \lambda_{\max}(\mathbf{H}_1(\lambda) - \text{diag}(\alpha')).$$

In the notation of (39),

$$F(\alpha, \lambda) \leq F_1(\alpha', \lambda).$$

Suppose now that we have equality: Then  $F(\alpha, \lambda) = F_1(\alpha', \lambda)$  is a simple eigenvalue of both  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$  and  $\mathbf{H}_1(\lambda) - \text{diag}(\alpha')$ . By [20, Theorem 2], it is then necessary that the vector

$$(g^\lambda(x_1, x_{m+1}), \dots, g^\lambda(x_m, x_{m+1}))^T$$

is orthogonal to the eigenfunction of  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$  corresponding to the eigenvalue  $F(\alpha, \lambda)$ . But both these vectors have all entries positive, so this cannot happen. Therefore

$$F(\alpha, \lambda) < F_1(\alpha', \lambda).$$

Inserting  $\lambda = \lambda_1(\Omega, X', \alpha')$  yields

$$F(\alpha, \lambda_1(\Omega, X', \alpha')) < 0.$$

Since  $\lambda \mapsto F(\alpha, \lambda)$  is strictly increasing (Proposition 4.38) and  $\lambda_1(\Omega, X, \alpha)$  is the unique solution of  $F(\alpha, \lambda) = 0$ , we must therefore have  $\lambda_1(\Omega, X', \alpha') < \lambda_1(\Omega, X, \alpha)$ .  $\square$

## 5 Faber-Krahn-type inequalities

Let  $\Omega \subset \mathbb{R}^d$ ,  $d \geq 1$  be open and bounded. Consider the following variational problem: Assuming that  $\Omega$  has fixed volume, choose  $\Omega$  so as to minimize the principal eigenvalue of the Dirichlet Laplacian in  $\Omega$  (recall Proposition 4.13). As explained in the introduction, this problem is solved by the *Faber-Krahn inequality*: With standard notation for the principal eigenvalues, we have

**Theorem 5.1** ([18, Theorem 3.2.1]). *Let  $B \subset \mathbb{R}^d$  be an open ball with the same volume (Lebesgue measure) as  $\Omega$ . Then*

$$\lambda_1(B) \leq \lambda_1(\Omega). \quad (41)$$

It obviously follows that the solution to the variational problem is  $\Omega = B$ . Our goal in the remaining few sections is to derive similar variational inequalities for point-interaction Hamiltonians in bounded domains, but we shall begin with a general operator-theoretic result.

### 5.1 The abstract case with defect indices (1,1)

Henceforth, assume  $d \in \{2, 3\}$  and that  $\Omega \subset \mathbb{R}^d$  is open, bounded, and connected with  $C^\infty$ -boundary. Recall the Faber-Krahn-type inequality (6), proven in [24]; in our notation, this inequality takes on the appearance

$$\lambda_1(B, \{0\}, \alpha) \leq \lambda_1(\Omega, \{x\}, \alpha) \quad \text{for all } x \in \Omega, \alpha \in \mathbb{R}. \quad (42)$$

One of the key insights of [24] was that this inequality follows essentially from a different inequality, namely *Bandle's inequality* for the relative Green's functions with respect to  $\Omega$  and  $B$ . In the authors' own words:

“It is admittedly remarkable that the estimate [...] involving Green functions of Dirichlet Laplacians, is so intimately connected with the spectral theory of the Hamiltonian with a point interaction in bounded domain.”

As we now show, this connection generalizes all the way to arbitrary densely defined lower semibounded operators with defect indices (1, 1). When attempting this generalization we immediately face two fundamental issues: First, we need a canonical way of parametrizing the self-adjoint extensions of the operators using real numbers, and second, we need to formulate an appropriate “abstract” Bandle's inequality for the operators. Both of these issues are solved by our theory of admissible operators. First, however, we need a lemma:

**Lemma 5.2.** *For  $i = 1, 2$  let  $a_i \in \mathbb{R}$  and let  $f_i : (-\infty, a_i) \rightarrow \mathbb{R}$  be a strictly increasing bijection. Then the following are equivalent:*

- (i)  $a_1 \leq a_2$  and  $f_1(x) \geq f_2(x)$  for all  $x < a_1$ ;
- (ii)  $f_1^{-1}(y) \leq f_2^{-1}(y)$  for all  $y \in \mathbb{R}$ .

We emphasize that  $f_1$  and  $f_2$  need to be bijections for this lemma to hold.

*Proof.* First suppose (i) holds. Let  $y \in \mathbb{R}$  and  $x_i := f_i^{-1}(y)$ ,  $i = 1, 2$ . Then  $x_1 < a_1 \leq a_2$ , and  $f_2(x_1) \leq f_1(x_1) = y = f_2(x_2)$ . Since  $f_2$  is strictly increasing, this implies  $x_1 \leq x_2$ . That is,  $f_1^{-1}(y) \leq f_2^{-1}(y)$ . Now suppose (ii) holds. Since  $f_i$ ,  $i = 1, 2$  are strictly increasing bijections,  $f_i^{-1} : \mathbb{R} \rightarrow (-\infty, a_i)$ ,  $i = 1, 2$  are strictly increasing bijections. Hence

$$a_1 = \lim_{y \rightarrow +\infty} f_1^{-1}(y) \leq \lim_{y \rightarrow +\infty} f_2^{-1}(y) = a_2.$$

Let  $x < a_1$ . Then  $x < a_2$  also, so we may let  $y_i := f_i(x)$ ,  $i = 1, 2$ . It follows that  $f_1^{-1}(y_1) = x = f_2^{-1}(y_2) \geq f_1^{-1}(y_2)$ . Since  $f_1^{-1}$  is strictly increasing, this implies  $y_1 \geq y_2$ . That is,  $f_1(x) \geq f_2(x)$ .  $\square$

Recall the notation and results in Section 3.7. In the next theorem, the inequality  $\mathbf{m}(T_1) \leq \mathbf{m}(T_2)$  takes the role of the Faber-Krahn inequality (41), the inequality between the Weyl primitives takes the role of Bandle's inequality (see the next section), and the inequality in (ii) takes the role of the Faber-Krahn-type inequality (42).

**Theorem 5.3.** *For  $i = 1, 2$ , let  $(T_i, \mathbb{E}_i, (\mathbf{w}_i))$  be an admissible operator such that  $T_i$  has defect indices  $(1, 1)$  and  $\mathbf{m}((T_i)_\alpha) < \mathbf{m}(T_i)$  for all  $\alpha \in \mathbb{R}$ . Then the following are equivalent:*

- (i)  $\mathbf{m}(T_1) \leq \mathbf{m}(T_2)$  and  $\mathbf{w}_1(\lambda) \geq \mathbf{w}_2(\lambda)$  for all  $\lambda < \mathbf{m}(T_1)$ ;
- (ii)  $\mathbf{m}((T_1)_\alpha) \leq \mathbf{m}((T_2)_\alpha)$  for all  $\alpha \in \mathbb{R}$ .

*Proof.* For  $i = 1, 2$ , our hypothesis together with Lemma 3.47 implies that the map  $\mathbf{w}_i : (-\infty, \mathbf{m}(T_i)) \rightarrow \mathbb{R}$  is a strictly increasing bijection, while Proposition 3.45 asserts that  $\alpha \mapsto \mathbf{m}((T_i)_\alpha)$  is the inverse of  $\mathbf{w}_i$ . We therefore only have to take  $a_i = \mathbf{m}(T_i)$  and  $f_i = \mathbf{w}_i$  in the above lemma.  $\square$

Note that the two operators  $T_i$ ,  $i = 1, 2$  in the theorem need not be defined in the same Hilbert space.

## 5.2 The one-point case for the Hamiltonian

As mentioned earlier, the relative Green's functions with respect to the domains  $\Omega$  and  $B$  are related by *Bandle's inequality*:

**Proposition 5.4.**  $h_\Omega^\lambda(x, x) \leq h_B^\lambda(0, 0)$  for all  $\lambda < \lambda_1(B)$ ,  $x \in \Omega$

The following proof has been adapted from that of [24, Proposition 2.6(iv)]. We have included it for the sake of completeness as it is not present in [4].

*Proof.* Let  $B(r)$  denote the open ball centered at the origin with radius  $r > 0$ . Let  $R$  be the radius of the open ball  $B$ . By [4, Lemma 2.3], there exists a unique  $R' \leq R$  such that  $h_{B(R')}^\lambda(0, 0) = h_\Omega^\lambda(x, x)$ . As is stated in the proof of the same

lemma, the map  $r \mapsto h_{B(r)}^\lambda(0, 0)$  is monotone increasing in the interval where  $g_{B(r)}^\lambda(\cdot, 0)$  is positive. In our case this interval is the whole positive real line, and since  $R' \leq R$ , we conclude that  $h_\Omega^\lambda(x, x) = h_{B(R')}^\lambda(0, 0) \leq h_{B(R)}^\lambda(0, 0) = h_B^\lambda(0, 0)$ .  $\square$

We can now recover the Faber-Krahn-type inequality (42) using only our operator-theoretic result from the previous section along with the Faber-Krahn and Bandle inequalities.

**Theorem 5.5.**  $\lambda_1(B, \{0\}, \alpha) \leq \lambda_1(\Omega, \{x\}, \alpha)$  for all  $x \in \Omega$ ,  $\alpha \in \mathbb{R}$ .

*Proof.* Theorem 4.30 furnishes two admissible operators  $(H_i, \mathbb{G}_i, \mathbf{H}_i)$ ,  $i = 1, 2$ , where  $(H_1, \mathbb{G}_1, \mathbf{H}_1)$  is constructed from the pair  $(B, \{0\})$  and  $(H_2, \mathbb{G}_2, \mathbf{H}_2)$  is constructed from the pair  $(\Omega, \{0\})$ . For  $i = 1, 2$ , the operator  $H_i$  has defect indices  $(1, 1)$  by Corollary 4.27, while Proposition 4.35 merely expresses that  $\mathfrak{m}((H_i)_\alpha) < \mathfrak{m}(H_i)$  for all  $\alpha \in \mathbb{R}$  but in a different notation. Thus all hypotheses of Theorem 5.3 are satisfied. The Faber-Krahn inequality (Theorem 5.1) is formulated in terms of the principal eigenvalues of the Dirichlet Laplacians  $-\Delta_D^B$  and  $-\Delta_D^\Omega$ , but these operators are exactly the Friedrichs extensions of the operators  $H_1$  and  $H_2$ , respectively (Proposition 4.25). Hence the Faber-Krahn inequality is equivalent to the inequality  $\mathfrak{m}(H_1) \leq \mathfrak{m}(H_2)$ . The Weyl primitives of the two admissible operators are  $\mathbf{H}_1(\lambda) = (h_B^\lambda(0, 0))$  and  $\mathbf{H}_2(\lambda) = (h_\Omega^\lambda(x, x))$ . It follows from Bandle's inequality (Proposition 5.4) that Theorem 5.3(i) holds, and therefore (ii), which is exactly the assertion, must also be true.  $\square$

### 5.3 The multi-point case for the Hamiltonian

Let  $X = \{x_1, x_2, \dots, x_m\}$  be a finite nonempty subset of  $\Omega$ . In this section we attempt to generalize Theorem 5.5 to the multi-point case. More specifically, we search for a function  $f_m : \mathbb{R}^m \rightarrow \mathbb{R}$  such that

$$\lambda_1(B, \{0\}, f_m(\alpha)) \leq \lambda_1(\Omega, X, \alpha) \quad \text{for all } \alpha \in \mathbb{R}^m. \quad (43)$$

The most natural suggestion might be  $f_m(\alpha) = \alpha_1 + \dots + \alpha_m$ , but this function is forbidden straight away by the next lemma.

**Lemma 5.6.** *Assume  $m \geq 2$ . If  $f_m$  satisfies (43), then  $f_m(\alpha)$  does not approach infinity as  $\alpha_i \rightarrow \infty$  for any  $i = 1, 2, \dots, m$ .*

*Proof.* Fix  $i$  and suppose for the sake of contradiction that

$$\lim_{\alpha_i \rightarrow \infty} f_m(\alpha) \rightarrow \infty.$$

Corollary 3.46 implies that  $\beta \mapsto \lambda_1(B, \{0\}, \beta)$  is a strictly increasing bijection of  $\mathbb{R}$  onto  $(-\infty, \lambda_1(B))$ , and consequently

$$\lim_{\alpha_i \rightarrow \infty} \lambda_1(B, \{0\}, f_m(\alpha)) = \lambda_1(B),$$

which by (43) implies that for any choice of  $\alpha_j \in \mathbb{R}$ ,  $j \in \{1, \dots, m\} \setminus \{i\}$ ,

$$\lim_{\alpha_i \rightarrow \infty} \lambda_1(\Omega, X, \alpha) \geq \lambda_1(B).$$

Moreover, successive applications of Theorem 4.41 implies that for each  $j$ ,

$$\lambda_1(\Omega, X, \alpha) < \lambda_1(\Omega, \{x_j\}, \alpha_j).$$

It follows that  $\lambda_1(B) \leq \lambda_1(\Omega, \{x_j\}, \alpha_j)$  for all  $\alpha_j \in \mathbb{R}$ ,  $j \neq i$ , but this contradicts the fact that  $\alpha_j \mapsto \lambda_1(\Omega, \{x_j\}, \alpha_j)$  is a bijection of onto  $(-\infty, \lambda_1(\Omega))$  and must assume values strictly below  $\lambda_1(B)$  for some choices of  $\alpha_j$ .  $\square$

When taking Lemma 5.6 into consideration, the second most natural suggestion might be  $f_m(\alpha) = \min_i \alpha_i$ . As Theorem 5.8 shows, this guess is almost correct except for a missing term inside the minimum.

Before proceeding we need another lemma. For each  $\lambda < \lambda_1(\Omega)$ , let  $g^\lambda$  be the Green's function of  $-\Delta - \lambda$  with respect to  $\Omega$  and let

$$G_i^\lambda := \sum_{j \neq i} g^\lambda(x_i, x_j) \quad \text{for } i = 1, 2, \dots, m. \quad (44)$$

Recall also the shorthand (39).

**Lemma 5.7.** *For all  $\alpha \in \mathbb{R}^m$  and  $\lambda < \lambda_1(\Omega)$ ,*

$$\min_i \{h^\lambda(x_i, x_i) - \alpha_i - G_i^\lambda\} \leq F(\alpha, \lambda) \leq \max_i \{h^\lambda(x_i, x_i) - \alpha_i + G_i^\lambda\}. \quad (45)$$

*Proof.* Let  $a_i := h^\lambda(x_i, x_i) - \alpha_i$  be the diagonal elements of  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$ . Note that  $G_i^\lambda$  is the sum of the absolute values of the nondiagonal elements of row  $i$  of  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$ . It follows by the Gershgorin circle theorem that each eigenvalue of  $\mathbf{H}(\lambda) - \text{diag}(\alpha)$  must lie within at least one of the  $m$  intervals  $[a_i - G_i^\lambda, a_i + G_i^\lambda]$ . Since  $F(\alpha, \lambda)$  is defined as the maximal eigenvalue, it must be less than or equal to the largest of the upper endpoints  $a_i + G_i^\lambda$ , which gives the upper bound. The lower bound is derived similarly.  $\square$

Without further ado we now state our Faber-Krahn-type inequality for multi-point interaction Hamiltonians, which to our knowledge is a novel result.

**Theorem 5.8.** *We have*

$$\lambda_1(B, \{0\}, \min_i \{\alpha_i - G_i^0\}) \leq \lambda_1(\Omega, X, \alpha) \quad (46)$$

for all  $\alpha \in \mathbb{R}^m$  such that  $\lambda_1(\Omega, X, \alpha) \leq 0$ .

*Proof.* Let  $\beta := \min_i \{\alpha_i - G_i^0\}$  and  $\lambda \leq 0$ . Let us also supplement our shorthand (39) with the domain  $\Omega$  and set  $X$  by writing  $F_{\Omega, X}(\alpha, \lambda)$  in order to show the

explicit dependence on these; then

$$\begin{aligned}
F_{\Omega, X}(\alpha, \lambda) &\leq \max_i \{h_{\Omega}^{\lambda}(x_i, x_i) - \alpha_i + G_i^{\lambda}\} \\
&\leq \max_i \{h_{\Omega}^{\lambda}(x_i, x_i) - \alpha_i + G_i^0\} \\
&\leq h_B^{\lambda}(0, 0) - \beta \\
&= F_{B, \{0\}}(\beta, \lambda)
\end{aligned} \tag{47}$$

where we have used (in order) Lemma 5.7, Proposition 4.22(iii), Bandle's inequality (Proposition 5.4), and (39) along with the fact that the maximal eigenvalue of a  $1 \times 1$ -matrix is equal to its only component. Taking  $\lambda = \lambda_1(\Omega, X, \alpha)$  therefore yields

$$0 \leq F_{B, \{0\}}(\beta, \lambda_1(\Omega, X, \alpha)).$$

Now we may argue as in the proof of Theorem 4.41: Since  $\lambda \mapsto F_{B, \{0\}}(\beta, \lambda)$  is strictly increasing (Proposition 4.38) and  $\lambda_1(B, \{0\}, \beta)$  is the unique solution of  $F_{B, \{0\}}(\beta, \lambda) = 0$ , the above inequality implies  $\lambda_1(B, \{0\}, \beta) \leq \lambda_1(\Omega, X, \alpha)$ .  $\square$

When comparing Theorem 5.5 and Theorem 5.8, we see that the latter contains an additional term  $G_i^0$  that does not appear in the former, and which moreover depends on both  $\Omega$  and  $X$  through the Green's functions in its definition (45). In dimension three we have the following bounds for this term:

**Proposition 5.9.** *Suppose  $d = 3$ . Then there exist positive constants  $K_1, K_2$  only dependent on the domain  $\Omega$  such that*

$$G_i^0 \leq K_1(m-1) \sum_{j \neq i} |x_i - x_j|^{-1}$$

and, for any  $i, j$  such that  $|x_i - x_j| \leq \frac{1}{2} \text{dist}(x_j, \partial\Omega)$ ,

$$G_i^0 \geq K_2 |x_i - x_j|^{-1}.$$

*Proof.* By [17, Theorem 1.2.5] there exists a constant  $K_1 > 0$  only dependent on  $\Omega$  such that  $g^0(x, y) \leq K_{\Omega} |x - y|^{-1}$  for all  $x, y \in \Omega$ ,  $x \neq y$ , which together with (44) yields the first inequality. The second constant and inequality follows similarly by [17, Theorem 1.2.5].  $\square$

Thus we see that  $G_i^0$  explodes as any pair of points in  $X$  approach each other, at least in dimension three. (The author could not find a similar inequality for the case  $d = 2$  and bounded domains.) Since the map  $\beta \mapsto \lambda_1(B, \{0\}, \beta)$  is strictly increasing (Theorem 4.39), this implies that the left-hand side of (46) decreases as any pair of points in  $X$  approach each other. This is a phenomenon that for obvious reasons does not occur in the one-point case.

A re-examination of the proof of Theorem 5.8 makes clear that the term  $G_i^0$  appears as a consequence of the very first inequality in (47) and that any improvement to the upper bound in Lemma 5.7 leads to a smaller gap in the inequality (46). The bounds in Lemma 5.7 were derived using the Gershgorin

circle theorem, which is valid for arbitrary complex matrices, so one might hope that by using more of the specific structure of  $\mathbf{H}(\lambda)$ , the upper bound could be improved sufficiently enough for the term  $G_i^\lambda$  to vanish. Unfortunately, as the next proposition shows, there exist certain choices of  $\Omega$  and  $X$  for which the upper bound in Lemma 5.7 is an equality.

**Proposition 5.10.** *Let  $\Omega$  be an open disc in  $\mathbb{R}^2$  and let  $x_1, x_2, \dots, x_m$  be equidistributed clockwise or counterclockwise on a circle contained inside and concentric to  $\Omega$ . Then*

$$F(\alpha, \dots, \alpha, \lambda) = h^\lambda(x_i, x_i) - \alpha + G_i^\lambda$$

for all  $\alpha \in \mathbb{R}$ ,  $\lambda < \lambda_1(\Omega)$ ,  $i = 1, 2, \dots, m$ .

*Proof.* The symmetry of  $\Omega$  implies that  $x \mapsto h^\lambda(x, x)$  is radially symmetric and therefore  $h^\lambda(x_i, x_i) = h^\lambda(x_1, x_1)$  for all  $i = 1, 2, \dots, m$ . Similarly, due to the symmetry of  $\Omega$  and the particular arrangement of the points  $x_1, x_2, \dots, x_m$ , we see that  $g^\lambda(x_i, x_j)$  only depends on the distance between  $x_i$  and  $x_j$ . This implies that for all  $i, j = 1, 2, \dots, m$  such that  $i \neq j$ ,

$$g^\lambda(x_i, x_j) = g^\lambda(x_{i+k \pmod{m}}, x_{j+k \pmod{m}}) \quad \text{for all } k \in \mathbb{Z}.$$

It follows that  $\mathbf{H}(\lambda) - \text{diag}(\alpha, \dots, \alpha)$  is a circulant matrix, i.e., for each  $i = 1, 2, \dots, m-1$  the  $(i+1)$ :th row of  $\mathbf{H}(\lambda) - \text{diag}(\alpha, \dots, \alpha)$  is obtained by cyclically permuting the  $i$ :th row one position to the right. Consequently  $\mathbf{u} = (1, 1, \dots, 1)^T$  is an eigenvector of  $\mathbf{H}(\lambda) - \text{diag}(\alpha, \dots, \alpha)$  with the row sum as its corresponding eigenvalue. (These sums are all equal since the matrix is circulant.) On the other hand, Proposition 4.36 implies that  $\mathbf{u}$  must be the eigenvector corresponding to  $F(\alpha, \lambda)$ , which proves the assertion.  $\square$

We conclude that for some triplets  $(\Omega, X, \alpha)$ , the very first inequality in (47) is actually an equality. Proceeding with Bandle's inequality is therefore guaranteed to add a term of the form  $G_i^\lambda$  in (46), at least if one finishes the proof as usual. Of course, there is still the possibility that there exist more sophisticated inequalities of, say, the form  $h_\Omega^\lambda(x_i, x_i) + G_i^\lambda \leq h_B^\lambda(y, y) + C$  that could be used to improve the first inequality and get rid of the extra term in (46) or possibly replace it with a better one, but at the time of writing the author is not aware of any such inequalities.

## 5.4 Failure of the strategy of test functions

Let  $d, \Omega, B, X$  all be as in the previous section. The authors' of [24] devised two rather different strategies for proving their Theorem 5.5: The first strategy is essentially the same as our proof and uses Bandle's inequality, except that they derived the necessary preparatory results (e.g. Proposition 3.45) only for single-point interaction Hamiltonians and by using other methods. (Indeed, our notion of admissible operators and Theorem 5.3 are direct results of our efforts to generalize this strategy.) Their second strategy is only sufficient to prove the

theorem for those  $\alpha \in \mathbb{R}$  such that  $\lambda_1(\Omega, \{0\}, \alpha) \geq 0$ , but it has the virtue of only requiring Bandle's inequality at  $\lambda = 0$ .

More specifically, their second strategy uses a test function approach along with the symmetric decreasing rearrangement, a.k.a. the Schwarz rearrangement (see the appendix for details). As our Theorem 5.8 does not have anything to say about the case  $\lambda_1(\Omega, X, \alpha) \geq 0$ , it was the hope of the author that this second strategy would generalize to the multi-point case. Though all necessary preparatory results ([24, Propositions 3.1, 3.2, 4.1]) have natural generalizations to the multi-point case, it unfortunately seems that the strategy falls just short of working. However, we believe it is of interest to include this admittedly negative result, as one of the original goals of this thesis was to see if the methods of [24] could be extended to the multi-point case.

First we need a lemma. Let  $g^\Omega$  (resp.  $g^B$ ) be the Green's function of  $-\Delta$  with respect to  $\Omega$  (resp. with respect to  $B$ ). As in the appendix, we use  $(g_x^\Omega)^*$  to denote the symmetric decreasing rearrangement of  $g_x^\Omega$ .

**Lemma 5.11.**  $(g_x^\Omega)^* \leq g_0^B$  for all  $x \in \Omega$ .

*Proof.* Recall Proposition 4.22(i) and take  $p \equiv 0$  in [4, Theorem 2.2].  $\square$

We now proceed with the strategy. Let  $\alpha \in \mathbb{R}^m$  and  $\beta := \min_i \{\alpha_i - G_i^0\}$ . Let  $\lambda := \lambda_1(\Omega, X, \alpha)$  and assume  $\lambda \geq 0$ . Let  $\mathbf{u}_\lambda$  be as in Theorem 4.39. Since obviously  $\mathbf{u}_\lambda \in \mathcal{D}(H_\alpha^{\Omega, X})$ , we know from the theory in Section 2.7 that

$$H_\alpha^{\Omega, X}[\mathbf{u}_\lambda] = \langle H_\alpha^{\Omega, X} \mathbf{u}_\lambda, \mathbf{u}_\lambda \rangle = \lambda \langle \mathbf{u}_\lambda, \mathbf{u}_\lambda \rangle = \lambda \|\mathbf{u}_\lambda\|_{L^2(\Omega)}^2.$$

Proposition 4.40 enables us to write  $\mathbf{u}_\lambda = f + \mathbf{u}_0$  for some  $f \in H_0^1(\Omega) \cap C(\bar{\Omega})$  such that  $f \geq 0$ , and hence

$$\lambda = \frac{H_\alpha^{\Omega, X}[f + \mathbf{u}_0]}{\|f + \mathbf{u}_0\|_{L^2(\Omega)}^2}. \quad (48)$$

The strategy in [24] was to estimate the numerator and denominator separately, so we attempt to do the same. Starting with the numerator, we see that taking  $\lambda = 0$  in Theorem 3.43(ii) yields

$$\begin{aligned} H_\alpha^{\Omega, X}[f + \mathbf{u}_0] &= (-\Delta_D^\Omega)[f] - \mathbf{u}^H(\mathbf{H}_{\Omega, X}(0) - \text{diag}(\alpha))\mathbf{u} \\ &\geq \|\nabla f\|_{L^2(\Omega)}^2 - F_{\Omega, X}(\alpha, 0)|\mathbf{u}|^2 \end{aligned}$$

where we have used Definition 4.12(ii) and the fact that

$$\frac{\mathbf{u}^H(\mathbf{H}_{\Omega, X}(0) - \text{diag}(\alpha))\mathbf{u}}{|\mathbf{u}|^2} \leq F_{\Omega, X}(\alpha, 0)$$

which follows because the left-hand side is a Rayleigh quotient. The Polya-Szego inequality (Theorem 5.13(iii)) gives

$$\|\nabla f\|_{L^2(\Omega)}^2 \geq \|\nabla f^*\|_{L^2(B)}^2$$

and we can argue as in (47) to derive the inequality

$$F_{\Omega, X}(\alpha, 0) \leq h_B^0(0, 0) - \beta$$

but a difference this time around is that we only need to use Bandle's inequality at  $\lambda = 0$ . By these bounds and another application of Theorem 3.43(ii),

$$\begin{aligned} H_{\alpha}^{\Omega, X}[f + \mathbf{u}_0] &\geq \|\nabla f^*\|_{L^2(B)}^2 - (h_B^0(0, 0) - \beta)|\mathbf{u}|^2 \\ &= H_{\beta}^{B, \{0\}}[f^* + |\mathbf{u}|g_0^B]. \end{aligned} \quad (49)$$

Let us next bound the denominator of (48). We first expand it as

$$\begin{aligned} \|f + \mathbf{u}_0\|_{L^2(\Omega)}^2 &= \langle f + \sum \mathbf{u}_i g_i^{\Omega}, f + \sum \mathbf{u}_i g_i^{\Omega} \rangle_{L^2(\Omega)} \\ &= \|f\|_{L^2(\Omega)}^2 + 2 \sum_i \mathbf{u}_i \langle f, g_i^{\Omega} \rangle_{L^2(\Omega)} + \sum_{ij} \mathbf{u}_i \mathbf{u}_j \langle g_i^{\Omega}, g_j^{\Omega} \rangle_{L^2(\Omega)}. \end{aligned}$$

(Recall that the  $\mathbf{u}_i$  are positive.) The squared norm in the second line is equal to  $\|f^*\|_{L^2(B)}^2$  by Theorem 5.13(i), while the inner products can be bounded using the Hardy-Littlewood inequality (Theorem 5.13(ii)) together with Lemma 5.11: Namely, we have

$$\langle f, g_i^{\Omega} \rangle_{L^2(\Omega)} \leq \langle f^*, (g_{x_i}^{\Omega})^* \rangle_{L^2(B)} \leq \langle f^*, g_0^B \rangle_{L^2(B)}$$

and

$$\langle g_i^{\Omega}, g_j^{\Omega} \rangle_{L^2(\Omega)} \leq \langle (g_{x_i}^{\Omega})^*, (g_{x_j}^{\Omega})^* \rangle_{L^2(B)} \leq \langle g_0^B, g_0^B \rangle_{L^2(B)}$$

for all  $i, j = 1, 2, \dots, m$ . Since each  $\mathbf{u}_i$  is positive we therefore have

$$\begin{aligned} \|f + \mathbf{u}_0\|_{L^2(\Omega)}^2 &\leq \|f^*\|_{L^2(\Omega)}^2 + 2 \sum_i \mathbf{u}_i \langle f^*, g_0^B \rangle_{L^2(B)} + \sum_{ij} \mathbf{u}_i \mathbf{u}_j \langle g_0^B, g_0^B \rangle_{L^2(B)} \\ &= \|f^* + (\sum \mathbf{u}_i)g_0^B\|_{L^2(B)}^2. \end{aligned} \quad (50)$$

We may now combine (48), (49), and (50) to arrive at the inequality

$$\lambda \geq \frac{H_{\alpha}^{B, \{0\}}[f^* + |\mathbf{u}|g_0^B]}{\|f^* + (\sum \mathbf{u}_i)g_0^B\|_{L^2(B)}^2}.$$

In the one-point case ( $m = 1$ ) we have  $\sum_i \mathbf{u}_i = \mathbf{u}_i = |\mathbf{u}|$ , so we obtain a test function  $u := f^* + \mathbf{u}_i g_0^B$  along with an inequality

$$\lambda_1(\Omega, X, \alpha) \geq \frac{H_{\beta}^{B, \{0\}}[u]}{\|u\|_{L^2(B)}^2}.$$

Corollary 2.8 implies that the the principal eigenvalue of  $H_{\beta}^{B, \{0\}}$  cannot exceed the right-hand side of the above inequality (hence the name ‘‘test function’’) and consequently

$$\lambda_1(\Omega, X, \alpha) \geq \lambda_1(B, \{0\}, \beta).$$

Here  $\beta = \min_i \{\alpha_i - C_i^0\} = \alpha_1$ , so we have recovered Theorem 5.5 for those  $\alpha \in \mathbb{R}$  such that  $\lambda_1(\Omega, X, \alpha) \geq 0$ . However, in the multi-point case ( $m > 1$ ) we instead have the strict inequality  $\sum_i \mathbf{u}_i > |\mathbf{u}|$  and therefore

$$\|f^* + (\sum \mathbf{u}_i)g_0^B\|_{L^2(B)}^2 > \|f^* + |\mathbf{u}|g_0^B\|_{L^2(B)}^2$$

which is the opposite estimation compared to what we want. Thus we cannot take  $f^* + |\mathbf{u}|g_0^B$  as test function and the strategy would appear to fail. (At least, at the time of writing the author has not found a workaround for this.)

## Appendix

Here we present some results which we feel do not fit in the rest of the text.

### 5.5 Holomorphic operator-valued functions

Let  $\mathcal{H}$  be a Hilbert space. There are various ways one can define the notion of a holomorphic operator-valued function with values in  $\mathcal{B}(\mathcal{H})$ , but the natural ones all turn out to be equivalent:

**Proposition 5.12.** *Let  $U \subset \mathbb{C}$  be open, and let  $T : U \rightarrow \mathcal{B}(\mathcal{H})$  be an operator-valued function. The following are equivalent:*

- (i)  $T$  is uniformly holomorphic, meaning there exists  $T' : U \rightarrow \mathcal{B}(\mathcal{H})$  such that for all  $z \in U$ ,

$$\lim_{w \rightarrow 0} \left\| \frac{T(z+w) - T(z)}{w} - T'(z) \right\| = 0.$$

- (ii)  $T$  is strongly holomorphic, meaning there exists  $T' : U \rightarrow \mathcal{B}(\mathcal{H})$  such that for all  $z \in U$ ,  $f \in \mathcal{H}$ ,

$$\lim_{w \rightarrow 0} \frac{T(z+w)f - T(z)f}{w} = T'(z)f.$$

- (iii)  $T$  is weakly holomorphic, meaning there exists  $T' : U \rightarrow \mathcal{B}(\mathcal{H})$  such that for all  $z \in U$ ,  $f, g \in \mathcal{H}$ ,

$$\frac{d}{dz} \langle T(z)f, g \rangle = \langle T'(z)f, g \rangle.$$

*Proof.* It is immediate that (i) implies (ii) and (ii) implies (iii). The implication from (iii) to (i) follows from [22, Theorem III.3.12], which is stated for Banach spaces.  $\square$

## 5.6 The symmetric decreasing (Schwarz) rearrangement

Let  $d \geq 2$  be an integer. Given any measurable subset  $E \subset \mathbb{R}^d$  with finite Lebesgue measure, its *symmetric rearrangement*  $E^*$  is defined as the open ball in  $\mathbb{R}^d$  centered at the origin with the same Lebesgue measure as  $E$ . Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  be a nonnegative measurable function. The measurable subsets

$$\{f > t\} := \{x \in \mathbb{R}^d : f(x) > t\} \quad \text{for } t > 0$$

are called the *level supersets* of  $f$ , and we say that  $f$  *vanishes at infinity* if each level superset has finite Lebesgue measure. Assuming now that  $f$  vanishes at infinity, we define its *symmetric decreasing rearrangement* as the nonnegative measurable function  $f^* : \mathbb{R}^d \rightarrow \mathbb{R}$  given by

$$f^*(x) := \int_0^\infty \chi_{\{f > t\}}(x) dt,$$

where  $\chi_{\{f > t\}}(x)$  denotes the characteristic (indicator) function of  $\{f > t\}$ . One can show that  $\text{supp } f \subset E$  implies  $\text{supp } f^* \subset E^*$  [24, Lemma 2.1].

When  $E$  is a measurable subset of  $\mathbb{R}^d$  with finite measure and  $f : E \rightarrow \mathbb{R}$  is a nonnegative measurable function, let  $\tilde{f} : \mathbb{R}^d \rightarrow \mathbb{R}$  be the nonnegative measurable function defined by

$$\tilde{f}(x) := \begin{cases} f(x) & \text{if } x \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Then  $\tilde{f}$  obviously vanishes at infinity since each of its level supersets is contained in  $E$ . In this case the symmetric decreasing rearrangement can be extended to  $f$  by defining  $f^* := (\tilde{f})^*$ . We have  $\text{supp } \tilde{f} \subset E$ , so a previous remark implies  $\text{supp } f^* \subset E^*$ , and hence the symmetric decreasing arrangement of  $f : E \rightarrow \mathbb{R}$  can be considered as a function  $f^* : E^* \rightarrow \mathbb{R}$ .

**Theorem 5.13** ([24, Corollary 2.3]). *Let  $\Omega \subset \mathbb{R}^d$  be a bounded domain with  $C^\infty$ -boundary. Let  $f, g : \Omega \rightarrow \mathbb{R}$  be nonnegative measurable functions. Then*

(i)  $\|f\|_{L^2(\Omega)} = \|f^*\|_{L^2(\Omega^*)}$ ;

(ii) the Hardy-Littlewood inequality holds:

$$\int_{\Omega} fg dx \leq \int_{\Omega^*} f^* g^* dx;$$

(iii) if  $f \in H_0^1(\Omega)$ , then  $f^* \in H_0^1(\Omega^*)$  and the Polya-Szego inequality holds:

$$\|\nabla f\|_{L^2(\Omega)} \geq \|\nabla f^*\|_{L^2(\Omega^*)}.$$

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