Appendix A

Boundary triplets and Weyl functions

A.1 Linear relations

Let $\mathcal{H}$ be a separable Hilbert space. A *(closed) linear relation* in $\mathcal{H}$ is a (closed) linear subspace in $\mathcal{H} \times \mathcal{H}$. The set of all closed linear relations is denoted by $\widetilde{\mathcal{C}}(\mathcal{H})$. Since every linear operator in $\mathcal{H}$ can be identified with its graph, the set of linear operators can be seen as a subset of all linear relations in $\mathcal{H}$. In particular, the set of closed linear operators $\mathcal{C}(\mathcal{H})$ is a subset of $\widetilde{\mathcal{C}}(\mathcal{H})$.

Recall that the domain, the range, the kernel and the multivalued part of a linear relation Θ are given, respectively, by

$$\begin{aligned} \operatorname{dom}(\Theta) &= \{f \in \mathcal{H} : \text{there exists } g \in \mathcal{H} \text{ such that } (f,g) \in \Theta\}, \\ \operatorname{ran}(\Theta) &= \{g \in \mathcal{H} : \text{there exists } f \in \mathcal{H} \text{ such that } (f,g) \in \Theta\}, \\ \ker(\Theta) &= \{f \in \mathcal{H} : (f,0) \in \Theta\}, \\ \operatorname{mul}(\Theta) &= \{g \in \mathcal{H} : (0,g) \in \Theta\}. \end{aligned}$$

The adjoint linear relation Θ^* is defined by

$$\Theta^* = \{(\tilde{f},\tilde{g}) \in \mathcal{H} \times \mathcal{H} : \langle g, \tilde{f}\rangle_{\mathcal{H}} = \langle f, \tilde{g}\rangle_{\mathcal{H}} \text{ for all } (f,g) \in \Theta\}.$$

Θ is called *symmetric* if $\Theta \subseteq \Theta^*$. If $\Theta = \Theta^*$, then it is called *self-adjoint*. Note that $\operatorname{mul}(\Theta)$ is orthogonal to $\operatorname{dom}(\Theta)$ if Θ is symmetric. For a closed symmetric Θ satisfying $\operatorname{mul}(\Theta) = \operatorname{mul}(\Theta^*)$ (the latter is further equivalent to the fact that Θ is densely defined on $\operatorname{mul}(\Theta)^\perp$), setting

$$\mathcal{H}_{\mathrm{op}} := \overline{\operatorname{dom}(\Theta)} = \operatorname{mul}(\Theta)^\perp,$$

we obtain the following orthogonal decomposition:

$$\Theta = \Theta_{\mathrm{op}} \oplus \Theta_\infty, \tag{A.1}$$

where $\Theta_\infty = \{0\} \times \operatorname{mul}(\Theta)$ and Θ_{op} is the graph of a closed symmetric linear operator in $\mathcal{H}_{\mathrm{op}}$, called the *operator part* of Θ. Notice that for non-closed symmetric linear relations the decomposition (A.1) may not hold true as the next example shows.

Example A.1. Let $\mathcal{H} = \mathcal{H}_{\mathrm{op}} \oplus \mathcal{M}$, where $\mathcal{H}_{\mathrm{op}}$ and $\mathcal{M}$ are closed infinite-dimensional subspaces. Suppose A_0 is a non-closed, densely defined symmetric operator in $\mathcal{H}_{\mathrm{op}}$ and $\mathcal{M}_0 \subsetneq \mathcal{M}$ a non-closed subspace such that $\overline{\mathcal{M}_0} = \mathcal{M}$. Let A be the closure of A_0, fix $f_0 \in \operatorname{dom}(A) \setminus \operatorname{dom}(A_0)$ and $g_0 \in \mathcal{M} \setminus \mathcal{M}_0$ and define

$$\mathbf{f}_0 = (f_0, g_0 + Af_0) \in \Theta := \operatorname{Gr}(A) \oplus (\{0\} \times \mathcal{M}),$$

where $\mathrm{Gr}(A)$ is the graph of A. Define the linear relation Θ_0 as the linear (non-closed) span of $\mathrm{Gr}(A_0) \oplus (\{0\} \times \mathcal{M}_0)$ and $\mathbf{f}_0$. Clearly, $\Theta_0 \subsetneq \Theta$ and hence it is symmetric. Moreover, by construction $\overline{\mathrm{dom}(\Theta_0)} = \mathrm{mul}(\Theta_0)^{\perp}$. However, (A.1) fails to hold for Θ_0. Indeed, if P_2 is the projection in $\mathcal{H} \times \mathcal{H}$ onto the second component and $P_{\mathcal{M}}$ is the projection in $\mathcal{H}$ onto $\mathcal{M}$, then (A.1) would imply $\mathcal{M}_0 = \mathrm{mul}(\Theta_0) = P_M P_2(\Theta_0)$. However,

$$g_0 = P_M(g_0 + Af_0) = P_M P_2 \mathbf{f}_0 \notin \mathcal{M}_0.$$

This is a clear contradiction to the definition of Θ_0.

The inverse of the linear relation Θ is given by

$$\Theta^{-1} = \{(g, f) \in \mathcal{H} \times \mathcal{H} : (f, g) \in \Theta\}.$$

The sum of linear relations Θ_1 and Θ_2 is defined by

$$\Theta_1 + \Theta_2 = \{(f, g_1 + g_2) : (f, g_1) \in \Theta_1,\ (f, g_2) \in \Theta_2\}.$$

Hence one can introduce the resolvent $(\Theta - z)^{-1}$ of the linear relation Θ, which is well defined for all $z \in \mathbb{C}$. However, the set of those $z \in \mathbb{C}$ for which $(\Theta - z)^{-1}$ is the graph of a closed bounded operator in $\mathcal{H}$ is called the *resolvent set* of Θ and is denoted by $\rho(\Theta)$. Its complement $\sigma(\Theta) = \mathbb{C} \setminus \rho(\Theta)$ is called the *spectrum* of Θ. If Θ is self-adjoint, then taking into account (A.1) we obtain

$$(\Theta - z)^{-1} = (\Theta_{\mathrm{op}} - z)^{-1} \oplus \mathbb{O}_{\mathrm{mul}(\Theta)}. \tag{A.2}$$

This immediately implies that $\rho(\Theta) = \rho(\Theta_{\mathrm{op}})$, $\sigma(\Theta) = \sigma(\Theta_{\mathrm{op}})$ and, moreover, one can introduce the spectral types of Θ as those of its operator part Θ_{op}. Let us mention that self-adjoint linear relations admit a very convenient representation, which was first observed by F. S. Rofe-Beketov [188] in the finite-dimensional case (see also [191, Exercises 14.9.3–4]).[1]

Proposition A.2. *Let C and D be closed bounded operators on $\mathcal{H}$ and*

$$\Theta_{C,D} := \{(f, g) \in \mathcal{H} \times \mathcal{H} : Cf = Dg\}.$$

Then $\Theta_{C,D}$ is self-adjoint if and only if

$$CD^* = DC^*, \quad \ker \begin{pmatrix} C & -D \\ D & C \end{pmatrix} = \{0\}. \tag{A.3}$$

The second condition in (A.3) is equivalent to $\mathrm{rank}(C|D) = \dim(\mathcal{H})$ *whenever* $\dim(\mathcal{H}) < \infty$.

[1] This representation was rediscovered later by many authors; in the context of self-adjoint vertex conditions for metric graphs, the reference usually goes to [150].

We also need the following definition. For a symmetric linear relation Θ in $\mathcal{H}$, its defect subspace at $z \in \mathbb{C}$ is defined by $\mathcal{N}_z(\Theta) = \ker(\Theta^* - z)$. The numbers

$$\mathrm{n}_\pm(\Theta) := \dim \mathcal{N}_{\pm\mathrm{i}}(\Theta) = \dim\ker(\Theta^* \mp \mathrm{i})$$

are called the deficiency indices of Θ.

Let us mention that the adjoint relation $\Theta_{C,D}^*$ to $\Theta_{C,D}$ is given by

$$\Theta_{C,D}^* = \overline{\{(D^* f, C^* f) : f \in \mathcal{H}\}}.$$

In particular, $\Theta_{C,D}^*$ is symmetric exactly when the first equality in (A.3) holds true. Moreover, in this case the deficiency indices are given by

$$\mathrm{n}_\pm(\Theta_{C,D}^*) = \dim\ker(C \mp \mathrm{i}D).$$

Further details and facts about linear relations in Hilbert spaces can be found in, e.g., [56, Chapter 6.1], [191, Chapter 14].

A.2 Boundary triplets and proper extensions

Let A be a densely defined closed symmetric operator in a separable Hilbert space $\mathfrak{H}$ with equal deficiency indices $\mathrm{n}_\pm(A) = \dim \mathcal{N}_{\pm\mathrm{i}} \le \infty$, $\mathcal{N}_z := \ker(A^* - z)$.

Definition A.3 ([86]). A triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is called *a boundary triplet* for the adjoint operator A^* if $\mathcal{H}$ is a Hilbert space and $\Gamma_0, \Gamma_1\colon \mathrm{dom}(A^*) \to \mathcal{H}$ are bounded linear mappings such that the abstract Green's identity

$$\langle A^* f, g\rangle_{\mathfrak{H}} - \langle f, A^* g\rangle_{\mathfrak{H}} = \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{H}} - \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathcal{H}}$$

holds for all $f, g \in \mathrm{dom}(A^*)$ and the mapping

$$\begin{aligned}\Gamma\colon \mathrm{dom}(A^*) &\to \mathcal{H} \times \mathcal{H},\\ f &\mapsto (\Gamma_0 f, \Gamma_1 f)\end{aligned}$$

is surjective.

A boundary triplet for A^* exists if and only if the deficiency indices of A are equal (see, e.g., [56, Proposition 7.4], [191, Proposition 14.5]). Moreover, $\mathrm{n}_\pm(A) = \dim(\mathcal{H})$ and $A = A^* \upharpoonright \ker(\Gamma)$. Note also that the boundary triplet for A^* is not unique.

An extension $\widetilde{A}$ of A is called *proper* if $\mathrm{dom}(A) \subset \mathrm{dom}(\widetilde{A}) \subset \mathrm{dom}(A^*)$. The set of all proper extensions is denoted by $\mathrm{Ext}(A)$.

Theorem A.4 ([55, 157]). *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*. Then the mapping Γ defines a bijective correspondence between* $\mathrm{Ext}(A)$ *and the set of all linear relations in $\mathcal{H}$:*

$$\Theta \mapsto A_\Theta := A^* \upharpoonright \{f \in \mathrm{dom}(A^*) : \Gamma f = (\Gamma_0 f, \Gamma_1 f) \in \Theta\}. \tag{A.4}$$

Moreover, the following holds:

(i) $A_\Theta^* = A_{\Theta^*}$.

(ii) $A_\Theta \in \mathcal{C}(\mathfrak{H})$ *if and only if* $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$.

(iii) A_Θ *is symmetric if and only if* Θ *is symmetric and* $\mathrm{n}_\pm(A_\Theta) = \mathrm{n}_\pm(\Theta)$ *holds. In particular,* A_Θ *is self-adjoint if and only if* Θ *is self-adjoint.*

(iv) *If* $A_\Theta = A_\Theta^*$ *and* $A_{\widetilde{\Theta}} = A_{\widetilde{\Theta}}^*$, *then for every* $p \in (0, \infty]$ *the following equivalence holds:*

$$(A_\Theta - \mathrm{i})^{-1} - (A_{\widetilde{\Theta}} - \mathrm{i})^{-1} \in \mathfrak{S}_p(\mathfrak{H}) \iff (\Theta - \mathrm{i})^{-1} - (\widetilde{\Theta} - \mathrm{i})^{-1} \in \mathfrak{S}_p(\mathcal{H}).$$

Notice that according to (A.2), a self-adjoint linear relation Θ is said to belong to the von Neumann–Schatten ideal $\mathfrak{S}_p$ if its operator part Θ_{op} belongs to $\mathfrak{S}_p(\mathcal{H}_{\mathrm{op}})$.

Remark A.5. The proof of Theorem A.4 (i)–(ii) can be found in [56, Proposition 7.8] and [191, Proposition 14.7], and statement (iii) was obtained in [157, Proposition 3], see also [56, Proposition 7.14].

A.3 Weyl functions and extensions of semibounded operators

With a boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ one can associate two linear operators

$$A_0 := A^* \upharpoonright \ker(\Gamma_0), \quad A_1 := A^* \upharpoonright \ker(\Gamma_1).$$

It is clear that (A.4) implies $A_0 = A_{\Theta_0}$ and $A_1 = A_{\Theta_1}$, where $\Theta_0 = \{0\} \times \mathcal{H}$ and $\Theta_1 = \mathcal{H} \times \{0\}$. Hence, by Theorem A.4 (iii), $A_0 = A_0^*$ and $A_1 = A_1^*$.

Definition A.6 ([55]). Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*. The operator-valued function $M \colon \rho(A_0) \to \mathcal{B}(\mathcal{H})$ defined by

$$M(z) := \Gamma_1(\Gamma_0 \upharpoonright \mathcal{N}_z)^{-1}, \quad z \in \rho(A_0),$$

is called *the Weyl function* corresponding to the boundary triplet Π.

The Weyl function is well defined and holomorphic on $\rho(A_0)$. Moreover, it is a Herglotz–Nevanlinna function (see [55, Section 1], [56, Section 7.4.2] and also [191, Section 14.5]). If $A_\Theta \in \mathrm{Ext}(A)$, then one has the *Krein resolvent formula* (see [55, Section 1], [56, Section 7.6.1])

$$(A_\Theta - z)^{-1} = (A_0 - z)^{-1} + \gamma(z)(\Theta - M(z))^{-1}\gamma(z^*)^* \tag{A.5}$$

for all $z \in \rho(A_\Theta) \cap \rho(A_0)$. Here

$$\gamma(z) := (\Gamma_0 \upharpoonright \mathcal{N}_z)^{-1}$$

is the so-called *γ-field*.

Assume now that $A \in \mathcal{C}(\mathfrak{H})$ is a *lower semibounded* operator, i.e., $A \geq a\,\mathrm{I}_{\mathfrak{H}}$ with some $a \in \mathbb{R}$. Let a_0 be the largest lower bound for A,

$$a_0 := \inf_{0 \neq f \in \mathrm{dom}(A)} \frac{\langle Af, f\rangle_{\mathfrak{H}}}{\|f\|^2_{\mathfrak{H}}}.$$

The Friedrichs extension of A is denoted by A_F. If $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for A^* such that $A_0 = A_F$, then the corresponding Weyl function M is holomorphic on $\mathbb{C} \setminus [a_0, \infty)$. Moreover, M is strictly increasing on $(-\infty, a_0)$ (that is, for all $x, y \in (-\infty, a_0)$, $M(x) - M(y)$ is positive definite whenever $x > y$) and the following strong resolvent limit exists (see [55])

$$M(a_0) := s - R - \lim_{x \uparrow a_0} M(x).$$

However, $M(a_0)$ is in general a closed linear relation, which is bounded from below.

Theorem A.7 ([55, 158]). *Let $A \geq a\,\mathrm{I}_{\mathfrak{H}}$ with some $a \geq 0$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* such that $A_0 = A_F$. Also, let $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ and let A_Θ be the corresponding self-adjoint extension* (A.4)*. If $M(a) \in \mathcal{B}(\mathcal{H})$, then:*

(i) $A_\Theta \geq a\,\mathrm{I}_{\mathfrak{H}}$ *if and only if* $\Theta - M(a) \geq \mathbb{O}_{\mathcal{H}}$.

(ii) $\kappa_-(A_\Theta - a\,\mathrm{I}) = \kappa_-(\Theta - M(a))$.

If additionally A is positive definite, that is, $a > 0$, then:

(iii) A_Θ *is positive definite if and only if* $\Theta(0) := \Theta - M(0)$ *is positive definite.*

(iv) *For every $p \in (0, \infty]$ the following equivalence holds:*

$$A_\Theta^- \in \mathfrak{S}_p(\mathfrak{H}) \iff \Theta(0)^- \in \mathfrak{S}_p(\mathcal{H}),$$

where $\Theta(0)^- := \Theta(0)^-_{\mathrm{op}} \oplus \Theta(0)_\infty$.

Remark A.8. For the proofs of (i) and (ii) consult [55, Theorems 5 and 6]; the proofs of (iii)–(iv) can be found in [158, Theorem 3]. If A is not positive definite, then "$\Leftrightarrow$" in Theorem A.7 (iv) is replaced by the implication "$\Leftarrow$".

We also need the next result (see [55, Theorem 3] and [56, Theorem 8.22]).

Theorem A.9 ([55]). *Assume the conditions of Theorem A.7. Then the following statements*

(i) $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ *is lower semibounded,*

(ii) A_Θ *is lower semibounded,*

are equivalent if and only if $M(x)$ tends uniformly to $-\infty$ as $x \to -\infty$, that is, for every $N > 0$ there exists $x_N < 0$ such that $M(x) < -N \cdot \mathrm{I}_{\mathcal{H}}$ for all $x < x_N$.

Implication (ii) $\Rightarrow$ (i) always holds true (cf. Theorem A.7 (i)), however, the validity of the converse implication requires that M tends uniformly to $-\infty$. Let us mention in this connection that the weak convergence of $M(x)$ to $-\infty$, i.e., the relation

$$\lim_{x\to-\infty} \langle M(x)h, h\rangle_{\mathcal{H}} = -\infty$$

holds for all $h \in \mathcal{H} \setminus \{0\}$ whenever $A_0 = A_F$. Moreover, this relation characterizes Weyl functions of the Friedrichs extension A_F among all non-negative (and even lower semibounded) self-adjoint extensions of A (see [55, Proposition 4]).

The next result establishes a connection between the essential spectra of A_Θ and Θ and also it can be seen as an improvement of Theorem A.7 (iv).

Theorem A.10 ([68]). *Let $A \geq a_0 I_{\mathfrak{H}} > 0$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* such that $A_0 = A_F$. Also, let M be the corresponding Weyl function and let $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ be such that $A_\Theta = A_\Theta^*$ is lower semibounded. Then the following equivalences hold:*

$$\begin{aligned}
\inf \sigma_{\text{ess}}(A_\Theta) \geq 0 &\iff \inf \sigma_{\text{ess}}(\Theta - M(0)) \geq 0,\\
\inf \sigma_{\text{ess}}(A_\Theta) > 0 &\iff \inf \sigma_{\text{ess}}(\Theta - M(0)) > 0,\\
\inf \sigma_{\text{ess}}(A_\Theta) = 0 &\iff \inf \sigma_{\text{ess}}(\Theta - M(0)) = 0.
\end{aligned}$$

A.4 Direct sums of boundary triplets

Let $\mathfrak{J}$ be a countably infinite index set. For each $j \in \mathfrak{J}$, let A_j be a closed densely defined symmetric operator in a Hilbert space $\mathfrak{H}_j$ such that

$$0 < \mathrm{n}_+(A_j) = \mathrm{n}_-(A_j) \leq \infty.$$

Also, let $\Pi_j = \{\mathcal{H}_j, \Gamma_{0,j}, \Gamma_{1,j}\}$ be a boundary triplet for the operator A_j^*, $j \in \mathfrak{J}$. In the Hilbert space $\mathfrak{H} := \bigoplus_{j\in\mathfrak{J}} \mathfrak{H}_j$, consider the operator $A := \bigoplus_{j\in\mathfrak{J}} A_j$, which is symmetric and $\mathrm{n}_+(A) = \mathrm{n}_-(A) = \infty$. Its adjoint is given by $A^* = \bigoplus_{j\in\mathfrak{J}} A_j^*$. Let us define a direct sum $\Pi := \bigoplus_{j\in\mathfrak{J}} \Pi_j$ of boundary triplets Π_j by setting

$$\mathcal{H} := \bigoplus_{j\in\mathfrak{J}} \mathcal{H}_j, \quad \Gamma_0 := \bigoplus_{j\in\mathfrak{J}} \Gamma_{0,j}, \quad \Gamma_1 := \bigoplus_{j\in\mathfrak{J}} \Gamma_{1,j}. \tag{A.6}$$

The next result provides several criteria for (A.6) to be a boundary triplet for the operator $A^* = \bigoplus_{j\in\mathfrak{J}} A_j^*$.

Theorem A.11 ([143]). *Let $A = \bigoplus_{j\in\mathfrak{J}} A_j$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be defined by (A.6). Then the following conditions are equivalent:*

(i) $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ *is a boundary triplet for the operator A^*.*

(ii) *The mappings Γ_0 and Γ_1 are bounded as mappings from* $\mathrm{dom}(A^*)$ *equipped with the graph norm to $\mathcal{H}$.*

(iii) *The Weyl functions M_j corresponding to the triplets Π_j, $j \in \mathfrak{J}$, satisfy the following condition:*

$$\sup_{j\in\mathfrak{J}} \big(\|M_j(\mathrm{i})\|_{\mathcal{H}_j} + \|(\operatorname{Im} M_j(\mathrm{i}))^{-1}\|_{\mathcal{H}_j}\big) < \infty.$$

(iv) *If in addition A is non-negative, then* (i)–(iii) *are further equivalent to*

$$\sup_{j\in\mathfrak{J}} \big(\|M_j(-1)\|_{\mathcal{H}_j} + \|M_j'(-1)\|_{\mathcal{H}_j} + \|(M_j'(-1))^{-1}\|_{\mathcal{H}_j}\big) < \infty. \quad \text{(A.7)}$$

Remark A.12. Theorem A.11 was proved in [143, Section 3], however, it is essentially contained in [156, Section 3].