Chapter 8

Schrödinger Operators on Bounded Domains

For the multi-dimensional Schrödinger operator $-\Delta + V$ with a bounded real potential V on a bounded domain $\Omega \subset \mathbb{R}^n$ with a C^2-smooth boundary a boundary triplet and a Weyl function will be constructed. The self-adjoint realizations of $-\Delta + V$ in $L^2(\Omega)$ and their spectral properties will be investigated. One of the main difficulties here is to provide trace mappings on the domain of the maximal realization, in such a way that the second Green identity remains valid in an appropriate form. It is necessary to introduce and study Sobolev spaces on the domain Ω and its boundary $\partial\Omega$, which will be done in Section 8.2; in this context also the rigged Hilbert spaces from Section 8.1 arise as Sobolev spaces and their duals. The minimal and maximal operators, and the Dirichlet and Neumann trace maps on the maximal domain will be discussed in Section 8.3, and in Section 8.4 a boundary triplet and Weyl function for the maximal operator associated with $-\Delta + V$ is provided. The self-adjoint realizations, their spectral properties, and some natural boundary conditions are also discussed in Section 8.4. The class of semibounded self-adjoint realizations of $-\Delta + V$ in $L^2(\Omega)$ and the corresponding semibounded forms are studied in Section 8.5. For this purpose a boundary pair which is compatible with the boundary triplet in Section 8.4 is provided. Orthogonal couplings of Schrödinger operators are treated in Section 8.6 for the model problem in which $\mathbb{R}^n$ decomposes into a bounded C^2-domain Ω_+ and an unbounded component $\Omega_- = \mathbb{R}^n \setminus \overline{\Omega}_+$. Finally, in Section 8.7 the more general setting of Schrödinger operators on bounded Lipschitz domains is briefly discussed.

8.1 Rigged Hilbert spaces

In this preparatory section the notion of rigged Hilbert spaces or Gelfand triples is briefly recalled. For this, let $\mathfrak{G}$ and $\mathfrak{H}$ be Hilbert spaces and assume that $\mathfrak{G}$ is densely and continuously embedded in $\mathfrak{H}$, that is, one has $\mathfrak{G} \subset \mathfrak{H}$ and the

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embedding operator $\iota : \mathfrak{G} \hookrightarrow \mathfrak{H}$ is continuous with dense range and $\ker \iota = \{0\}$. In the following the dual space $\mathfrak{H}'$ is identified with $\mathfrak{H}$, but the dual space $\mathfrak{G}'$ of antilinear continuous functionals is not identified with $\mathfrak{G}$. Instead, the isometric isomorphism

$$\mathfrak{I} : \mathfrak{G}' \to \mathfrak{G}, \quad g' \mapsto \mathfrak{I}g', \quad \text{where} \quad (\mathfrak{I}g', g)_{\mathfrak{G}} = g'(g), \quad g \in \mathfrak{G}, \tag{8.1.1}$$

is written explicitly whenever used. In fact, in this section the continuous (antilinear) functionals on $\mathfrak{G}$ will be identified via the scalar product in $\mathfrak{H}$. In the following usually the notation

$$\langle g', g \rangle_{\mathfrak{G}' \times \mathfrak{G}} := g'(g) \tag{8.1.2}$$

is employed for the (antilinear) dual pairing in (8.1.1), and when no confusion can arise the index is suppressed, that is, one writes $\langle g', g \rangle = g'(g)$ for (8.1.2).

In the above setting the dual operator of the embedding operator $\iota : \mathfrak{G} \hookrightarrow \mathfrak{H}$ is given by

$$\iota' : \mathfrak{H} \hookrightarrow \mathfrak{G}', \quad (\iota' h)(g) = (h, \iota g)_{\mathfrak{H}}, \quad g \in \mathfrak{G}, \tag{8.1.3}$$

and in terms of the pairing $\langle \cdot, \cdot \rangle$ this means

$$\langle \iota' h, g \rangle = (h, \iota g)_{\mathfrak{H}}, \qquad h \in \mathfrak{H}, \ g \in \mathfrak{G}. \tag{8.1.4}$$

Since the scalar product $(\cdot, \cdot)_{\mathfrak{H}}$ is antilinear in the second argument one has $\langle \iota' h, \lambda g \rangle = \bar{\lambda} \langle \iota' h, g \rangle$ for $\lambda \in \mathbb{C}$, and hence $\iota' h$ is indeed antilinear. Observe that the dual operator ι' in (8.1.3) is continuous since ι is continuous. Moreover, from the identity $\ker \iota' = (\operatorname{ran} \iota)^{\perp_{\mathfrak{H}}}$ it follows that ι' is injective, and the range of ι' is dense in $\mathfrak{G}'$ since $\ker \iota'' = (\operatorname{ran} \iota')^{\perp_{\mathfrak{G}'}}$ and $\iota = \iota''$ as $\mathfrak{G}$ is reflexive. Thus,

$$\mathfrak{G} \overset{\iota}{\hookrightarrow} \mathfrak{H} \overset{\iota'}{\hookrightarrow} \mathfrak{G}' \quad \text{with } \operatorname{ran} \iota \subset \mathfrak{H} \text{ dense and } \operatorname{ran} \iota' \subset \mathfrak{G}' \text{ dense},$$

and since $\mathfrak{G}$ can be viewed as a subspace of $\mathfrak{H}$, and $\mathfrak{H}$ can be viewed as a subspace of $\mathfrak{G}'$, instead of (8.1.4) also the notation

$$\langle h, g \rangle = (h, g)_{\mathfrak{H}}, \qquad h \in \mathfrak{H}, \ g \in \mathfrak{G}, \tag{8.1.5}$$

will be used. The present situation will appear naturally in the context of Sobolev spaces later in this chapter. First the terminology will be fixed in the next definition.

Definition 8.1.1. Let $\mathfrak{G}$ and $\mathfrak{H}$ be Hilbert spaces such that $\mathfrak{G}$ is densely and continuously embedded in $\mathfrak{H}$. Then the triple $\{\mathfrak{G}, \mathfrak{H}, \mathfrak{G}'\}$ is a called a *Gelfand triple* or a *rigged Hilbert space*.

Assume now that $\{\mathfrak{G}, \mathfrak{H}, \mathfrak{G}'\}$ is a Gelfand triple. Since the embedding operator $\iota : \mathfrak{G} \hookrightarrow \mathfrak{H}$ is continuous, one has $\|g\|_{\mathfrak{H}} \le C \|g\|_{\mathfrak{G}}$ for all $g \in \mathfrak{G}$ with the constant

$C = \|\iota\| > 0$. Moreover, as $\mathfrak{G}$ is a Hilbert space it follows from Lemma 5.1.9 that the symmetric form

$$\mathfrak{t}[g_1, g_2] := (g_1, g_2)_{\mathfrak{G}}, \quad \operatorname{dom} \mathfrak{t} = \mathfrak{G},$$

is densely defined and closed in $\mathfrak{H}$ with a positive lower bound. Hence, by the first representation theorem (Theorem 5.1.18) there exists a unique self-adjoint operator T with the same positive lower bound in $\mathfrak{H}$, such that $\operatorname{dom} T \subset \operatorname{dom} \mathfrak{t}$ and

$$(g_1, g_2)_{\mathfrak{G}} = \mathfrak{t}[g_1, g_2] = (Tg_1, g_2)_{\mathfrak{H}}, \qquad g_1 \in \operatorname{dom} T,\ g_2 \in \mathfrak{G}.$$

Moreover, if $R := T^{\frac{1}{2}}$, then the second representation theorem (Theorem 5.1.23) implies $\operatorname{dom} R = \operatorname{dom} \mathfrak{t}$ and

$$(g_1, g_2)_{\mathfrak{G}} = \mathfrak{t}[g_1, g_2] = (Rg_1, Rg_2)_{\mathfrak{H}}, \qquad g_1, g_2 \in \operatorname{dom} R = \mathfrak{G}. \tag{8.1.6}$$

Note that R is a uniformly positive self-adjoint operator in $\mathfrak{H}$.

In the next lemma some more properties of the Gelfand triple $\{\mathfrak{G}, \mathfrak{H}, \mathfrak{G}'\}$ and the operator R are collected.

Lemma 8.1.2. *Let $\{\mathfrak{G}, \mathfrak{H}, \mathfrak{G}'\}$ be a Gelfand triple, let $\mathfrak{I} : \mathfrak{G}' \to \mathfrak{G}$ be the isometric isomorphism in (8.1.1), and let R be the uniformly positive self-adjoint operator in $\mathfrak{H}$ such that (8.1.6) holds. Then the following statements hold:*

(i) *The Hilbert space $\mathfrak{G}'$ coincides with the completion of $\mathfrak{H}$ equipped with the inner product $(R^{-1}\cdot, R^{-1}\cdot)_{\mathfrak{H}}$.*

(ii) *The operators $\iota_+ = R : \mathfrak{G} \to \mathfrak{H}$ and $\iota_- = R\mathfrak{I} : \mathfrak{G}' \to \mathfrak{H}$ are isometric isomorphisms such that*

$$(\iota_- g', \iota_+ g)_{\mathfrak{H}} = \langle g', g \rangle, \qquad g \in \mathfrak{G},\ g' \in \mathfrak{G}'. \tag{8.1.7}$$

(iii) *For all $h \in \mathfrak{H}$ one has $\iota_- h = R^{-1} h$.*

(iv) *For all $h \in \mathfrak{H}$ and $g \in \mathfrak{G}$ one has $\iota_+ \iota_- h = h$ and $\iota_- \iota_+ g = g$.*

(v) *The operator R^{-2} can be extended by continuity to an isometric operator $\widetilde{R}^{-2} : \mathfrak{G}' \to \mathfrak{G}$ which coincides with the isometric isomorphism $\mathfrak{I} : \mathfrak{G}' \to \mathfrak{G}$.*

Proof. (i) Consider an element $g' \in \mathfrak{G}'$ and assume, in addition, that $g' \in \mathfrak{H}$. Then one has

$$\|g'\|_{\mathfrak{G}'} = \sup_{g \in \mathfrak{G} \setminus \{0\}} \frac{|g'(g)|}{\|g\|_{\mathfrak{G}}} = \sup_{g \in \mathfrak{G} \setminus \{0\}} \frac{|\langle g', g \rangle|}{\|g\|_{\mathfrak{G}}} = \sup_{g \in \mathfrak{G} \setminus \{0\}} \frac{|(g', g)_{\mathfrak{H}}|}{\|g\|_{\mathfrak{G}}},$$

where (8.1.2) was used in the second equality, and $g' \in \mathfrak{H}$ and (8.1.5) were used in the last step. Since R is uniformly positive, one has $R^{-1} \in \mathbf{B}(\mathfrak{H})$, and using (8.1.6) one obtains

$$\|g'\|_{\mathfrak{G}'} = \sup_{g \in \mathfrak{G} \setminus \{0\}} \frac{|(R^{-1} g', Rg)_{\mathfrak{H}}|}{\|Rg\|_{\mathfrak{H}}} = \sup_{h \in \mathfrak{H} \setminus \{0\}} \frac{|(R^{-1} g', h)_{\mathfrak{H}}|}{\|h\|_{\mathfrak{H}}} = \|R^{-1} g'\|_{\mathfrak{H}}.$$

Therefore, $\|g'\|_{\mathfrak{G}'} = \|R^{-1}g'\|_{\mathfrak{H}}$ for all $g' \in \mathfrak{H} \subset \mathfrak{G}'$ and as $\mathfrak{H}$ is dense in $\mathfrak{G}'$ with respect to the norm $\|\cdot\|_{\mathfrak{G}'}$, one concludes that $\mathfrak{G}'$ coincides with the completion of $\mathfrak{H}$ with respect to the norm $\|R^{-1}\cdot\|_{\mathfrak{H}}$.

(ii) Observe that by the definition of ι_+ and (8.1.6) one has

$$\|\iota_+ g\|_{\mathfrak{H}} = \|Rg\|_{\mathfrak{H}} = \|g\|_{\mathfrak{G}}, \quad g \in \mathfrak{G} = \operatorname{dom} \iota_+ = \operatorname{dom} R,$$

and hence $\iota_+ : \mathfrak{G} \to \mathfrak{H}$ is isometric. Moreover, since R is bijective, it follows that ι_+ is an isometric isomorphism. Similarly, for $g' \in \mathfrak{G}'$ one has

$$\|\iota_- g'\|_{\mathfrak{H}} = \|R\mathfrak{I}g'\|_{\mathfrak{H}} = \|\mathfrak{I}g'\|_{\mathfrak{G}} = \|g'\|_{\mathfrak{G}'},$$

where in the last step it was used that $\mathfrak{I} : \mathfrak{G}' \to \mathfrak{G}$ is an isometric isomorphism. In order to check the identity (8.1.7), let $g' \in \mathfrak{G}'$ and $g \in \mathfrak{G}$. Then (8.1.6) and (8.1.1) imply

$$(\iota_- g', \iota_+ g)_{\mathfrak{H}} = (R\mathfrak{I}g', Rg)_{\mathfrak{H}} = (\mathfrak{I}g', g)_{\mathfrak{G}} = \langle g', g\rangle. \tag{8.1.8}$$

(iii) Let $g' \in \mathfrak{H} \subset \mathfrak{G}'$ and $g \in \mathfrak{G}$. By (8.1.5), one has

$$\langle g', g\rangle = (g', g)_{\mathfrak{H}} = (R^{-1}g', Rg)_{\mathfrak{H}} = (R^{-1}g', \iota_+ g)_{\mathfrak{H}}$$

and comparing this with (8.1.8) it follows that $R^{-1}g' = \iota_- g'$ for all $g' \in \mathfrak{H}$.

(iv) By the definition of ι_+ and (iii) it is clear that $\iota_+\iota_- h = RR^{-1}h = h$. Similarly, $\iota_-\iota_+ g = \iota_- Rg = R^{-1}Rg = g$ for $g \in \mathfrak{G}$ by (iii).

(v) For $h \in \mathfrak{H}$ one has $\|R^{-2}h\|_{\mathfrak{G}} = \|R^{-1}h\|_{\mathfrak{H}} = \|h\|_{\mathfrak{G}'}$ by (8.1.6) and (i), and since $\mathfrak{H}$ is dense in $\mathfrak{G}'$, it follows that R^{-2} admits an extension to an isometric operator $\widetilde{R}^{-2} : \mathfrak{G}' \to \mathfrak{G}$. Moreover, for $h \in \mathfrak{H}$ it follows from the definition of ι_- in (ii) and (iii) that

$$R\mathfrak{I}h = \iota_- h = R^{-1}h, \quad \text{and hence} \quad \mathfrak{I}h = R^{-2}h.$$

Thus $\mathfrak{I}$ and the restriction R^{-2} of $\widetilde{R}^{-2}$ coincide on the dense subspace $\mathfrak{H} \subset \mathfrak{G}'$. This implies $\mathfrak{I} = \widetilde{R}^{-2}$. □

Now a different point of view is taken on Gelfand triples. In the next lemma it is shown that the powers R^s for $s \geq 0$ of a uniformly positive self-adjoint operator R in $\mathfrak{H}$ give rise to Gelfand triples with certain compatibility properties.

Lemma 8.1.3. *Let $\mathfrak{H}$ be a Hilbert space and let R be a uniformly positive self-adjoint operator R in $\mathfrak{H}$. Let $s \geq 0$ and equip $\mathfrak{G}_s := \operatorname{dom} R^s$ with the inner product*

$$(h, k)_{\mathfrak{G}_s} := (R^s h, R^s k)_{\mathfrak{H}}, \qquad h, k \in \operatorname{dom} R^s. \tag{8.1.9}$$

Then $\mathfrak{G}_t \subset \mathfrak{G}_s$ for all $t \geq s \geq 0$ and the following statements hold:

(i) *$\{\mathfrak{G}_s, \mathfrak{H}, \mathfrak{G}'_s\}$ is a Gelfand triple and the assertions in Lemma 8.1.2 hold with R, $\mathfrak{G}$, and $\mathfrak{G}'$ replaced by R^s, $\mathfrak{G}_s$, and $\mathfrak{G}'_s$, respectively.*

(ii) *If* $\iota_+ : \mathfrak{G}_1 \to \mathfrak{H}$ *and* $\iota_- : \mathfrak{G}_1' \to \mathfrak{H}$ *denote the isometric isomorphisms corresponding to the Gelfand triple* $\{\mathfrak{G}_1, \mathfrak{H}, \mathfrak{G}_1'\}$ *such that*

$$(\iota_- g', \iota_+ g)_{\mathfrak{H}} = \langle g', g\rangle_{\mathfrak{G}_1' \times \mathfrak{G}_1}, \quad g' \in \mathfrak{G}_1',\, g \in \mathfrak{G}_1,$$

then their restrictions

$$\iota_+ = R : \mathfrak{G}_{s+1} \to \mathfrak{G}_s \quad \textit{and} \quad \iota_- = R^{-1} : \mathfrak{G}_s \to \mathfrak{G}_{s+1}, \quad s \geq 0, \tag{8.1.10}$$

are isometric isomorphisms such that $\iota_+\iota_- g = g$ *for* $g \in \mathfrak{G}_s$ *and* $\iota_-\iota_+ l = l$ *for* $l \in \mathfrak{G}_{s+1}$.

Proof. (i) For $s \geq 0$ the self-adjoint operator R^s is uniformly positive in $\mathfrak{H}$ and hence $\mathfrak{G}_s = \operatorname{dom} R^s$ equipped with the inner product (8.1.9) is a Hilbert space which is dense in $\mathfrak{H}$. Moreover, from $R^{-s} \in \mathbf{B}(\mathfrak{H})$ and (8.1.9) one obtains that

$$\|g\|_{\mathfrak{H}} = \|R^{-s}R^s g\|_{\mathfrak{H}} \leq \|R^{-s}\|\|R^s g\|_{\mathfrak{H}} = \|R^{-s}\|\|g\|_{\mathfrak{G}_s}, \quad g \in \mathfrak{G}_s,$$

which shows that the embedding $\mathfrak{G}_s \hookrightarrow \mathfrak{H}$ is continuous. Therefore, if $\mathfrak{G}_s'$ denotes the dual of $\mathfrak{G}_s$, then $\{\mathfrak{G}_s, \mathfrak{H}, \mathfrak{G}_s'\}$ is a Gelfand triple. Comparing (8.1.9) with (8.1.6) shows that the operator R^s plays the same role as the representing operator of the inner product in (8.1.6). Hence, the assertions of Lemma 8.1.2 are valid with R, $\mathfrak{G}$, and $\mathfrak{G}'$ replaced by R^s, $\mathfrak{G}_s$, and $\mathfrak{G}_s'$, respectively.

(ii) Let $s \geq 0$ and consider $l \in \mathfrak{G}_{s+1} = \operatorname{dom} R^{s+1}$. It follows from (8.1.9) that

$$\|Rl\|_{\mathfrak{G}_s} = \|R^s R l\|_{\mathfrak{H}} = \|R^{s+1} l\|_{\mathfrak{H}} = \|l\|_{\mathfrak{G}_{s+1}}$$

and hence $\iota_+ = R : \mathfrak{G}_{s+1} \to \mathfrak{G}_s$ is isometric. In order to verify that this mapping is onto let $k \in \mathfrak{G}_s$. Then $k \in \mathfrak{H}$, and as R is bijective, there exists $l \in \operatorname{dom} R$ such that $Rl = k$. Therefore, $l = R^{-1}k$ and as $k \in \mathfrak{G}_s = \operatorname{dom} R^s$ one concludes $l \in \operatorname{dom} R^{s+1} = \mathfrak{G}_{s+1}$. This shows that $\iota_+ = R : \mathfrak{G}_{s+1} \to \mathfrak{G}_s$ is an isometric isomorphism for $s \geq 0$. A similar reasoning shows that $\iota_- = R^{-1} : \mathfrak{G}_s \to \mathfrak{G}_{s+1}$ is an isometric isomorphism for $s \geq 0$. The remaining assertions $\iota_+\iota_- g = g$ for $g \in \mathfrak{G}_s$ and $\iota_-\iota_+ l = l$ for $l \in \mathfrak{G}_{s+1}$ follow immediately from (8.1.10). □

8.2 Sobolev spaces, C^2-domains, and trace operators

In this section Sobolev spaces on $\mathbb{R}^n$, open subsets $\Omega \subset \mathbb{R}^n$, and on the boundaries $\partial\Omega$ of C^2-domains are defined and some of their features are briefly recalled. Furthermore, the mapping properties of the Dirichlet and Neumann trace map on a C^2-domain Ω are recalled and the first Green identity is established.

For $s \geq 0$ the scale of L^2-based Sobolev spaces $H^s(\mathbb{R}^n)$ is defined with the help of the (classical) Fourier transform $\mathcal{F} \in \mathbf{B}(L^2(\mathbb{R}^n))$ by

$$H^s(\mathbb{R}^n) := \bigl\{ f \in L^2(\mathbb{R}^n) : (1 + |\cdot|^2)^{s/2}\mathcal{F}f \in L^2(\mathbb{R}^n) \bigr\}$$

and $H^s(\mathbb{R}^n)$ is equipped with the natural norm

$$\|f\|_{H^s(\mathbb{R}^n)} := \big\|(1+|\cdot|^2)^{s/2}\mathcal{F}f\big\|_{L^2(\mathbb{R}^n)}, \qquad f \in H^s(\mathbb{R}^n),$$

and corresponding scalar product

$$(f,g)_{H^s(\mathbb{R}^n)} := \big((1+|\cdot|^2)^{s/2}\mathcal{F}f, (1+|\cdot|^2)^{s/2}\mathcal{F}g\big)_{L^2(\mathbb{R}^n)}, \quad f,g \in H^s(\mathbb{R}^n).$$

Then the space $H^s(\mathbb{R}^n)$ is a separable Hilbert space for every $s \geq 0$ and one has $H^0(\mathbb{R}^n) = L^2(\mathbb{R}^n)$. It is also useful to note that the space $C_0^\infty(\mathbb{R}^n)$ is dense in $H^s(\mathbb{R}^n)$ for all $s \geq 0$. Since the Fourier transform is a unitary operator in $L^2(\mathbb{R}^n)$, it is clear that

$$\mathcal{R} = \mathcal{F}^{-1}(1+|\cdot|^2)^{1/2}\mathcal{F}$$

is a uniformly positive self-adjoint operator in $L^2(\mathbb{R}^n)$ such that $\operatorname{dom}\mathcal{R} = H^1(\mathbb{R}^n)$. Furthermore, for each $s \geq 0$ one has

$$\mathcal{R}^s = \mathcal{F}^{-1}(1+|\cdot|^2)^{s/2}\mathcal{F}$$

and hence $\mathcal{R}^s$ for $s \geq 0$ is also a uniformly positive self-adjoint operator in $L^2(\mathbb{R}^n)$ such that $\operatorname{dom}\mathcal{R}^s = H^s(\mathbb{R}^n)$. Note that the scalar product in $H^s(\mathbb{R}^n)$ satisfies

$$(f,g)_{H^s(\mathbb{R}^n)} = (\mathcal{R}^s f, \mathcal{R}^s g)_{L^2(\mathbb{R}^n)}, \qquad f,g \in H^s(\mathbb{R}^n),$$

for all $s \geq 0$. In particular, $\mathcal{R}$ plays the same role as the operator R in (8.1.6) and $\mathcal{R}^s$ plays the same role as the operator R^s in (8.1.9). Hence, $\mathcal{R}^s$, $s \geq 0$, gives rise to a Gelfand triple $\{H^s(\mathbb{R}^n), L^2(\mathbb{R}^n), H^{-s}(\mathbb{R}^n)\}$, where $H^{-s}(\mathbb{R}^n)$ denotes the dual space consisting of continuous antilinear functionals on $H^s(\mathbb{R}^n)$. From Lemma 8.1.3 it is now clear that the restrictions $\mathcal{R} : H^{s+1}(\mathbb{R}^n) \to H^s(\mathbb{R}^n)$ and $\mathcal{R}^{-1} : H^s(\mathbb{R}^n) \to H^{s+1}(\mathbb{R}^n)$ are isometric isomorphisms for $s \geq 0$.

For a nonempty open subset $\Omega \subset \mathbb{R}^n$ and $s \geq 0$ define

$$H^s(\Omega) := \big\{f \in L^2(\Omega) : \text{there exists } g \in H^s(\mathbb{R}^n) \text{ such that } f = g|_\Omega\big\}$$

and endow this space with the norm

$$\|f\|_{H^s(\Omega)} := \inf_{\substack{g \in H^s(\mathbb{R}^n)\\ f = g|_\Omega}} \|g\|_{H^s(\mathbb{R}^n)}, \qquad f \in H^s(\Omega). \tag{8.2.1}$$

The space $H^s(\Omega)$ is a separable Hilbert space; the corresponding scalar product will be denoted by $(\cdot,\cdot)_{H^s(\Omega)}$. For $s \geq 0$ the space $C^\infty(\overline{\Omega}) := \{\varphi|_\Omega : \varphi \in C_0^\infty(\mathbb{R}^n)\}$ is dense in $H^s(\Omega)$. The closure of $C_0^\infty(\Omega)$ in $H^s(\Omega)$ is a closed subspace of $H^s(\Omega)$; it is denoted by

$$H_0^s(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{H^s(\Omega)}}. \tag{8.2.2}$$

In order to define Sobolev spaces on the boundary $\partial\Omega$ of some domain $\Omega \subset \mathbb{R}^n$ assume first that $\phi : \mathbb{R}^{n-1} \to \mathbb{R}$ is a C^2-function. The vectors in $\mathbb{R}^{n-1}$ will be denoted by $x' = (x_1, \dots, x_{n-1})^\top \in \mathbb{R}^{n-1}$ and the notation $(x', x_n)^\top$ is used for $(x_1, \dots, x_n)^\top \in \mathbb{R}^n$. Then the domain

$$\Omega_\phi := \{(x', x_n)^\top \in \mathbb{R}^n : x_n < \phi(x')\} \tag{8.2.3}$$

is called a C^2-*hypograph* and its boundary is given by

$$\partial\Omega_\phi = \{(x', \phi(x'))^\top \in \mathbb{R}^n : x' \in \mathbb{R}^{n-1}\}.$$

For a measurable function $h : \partial\Omega_\phi \to \mathbb{C}$ the surface integral on $\partial\Omega_\phi$ is defined as

$$\int_{\partial\Omega_\phi} h \, d\sigma := \int_{\mathbb{R}^{n-1}} h(x', \phi(x'))\sqrt{1 + |\nabla\phi(x')|^2}\, dx'. \tag{8.2.4}$$

If $\mathbf{1}_B$ denotes the characteristic function of a Borel set $B \subset \partial\Omega_\phi$, then the surface integral in (8.2.4) induces a surface measure

$$\sigma(B) = \int_{\partial\Omega_\phi} \mathbf{1}_B \, d\sigma. \tag{8.2.5}$$

This surface measure also gives rise to the usual L^2-space on $\partial\Omega_\phi$, which will be denoted by $L^2(\partial\Omega_\phi)$. Furthermore, for $s \in [0, 2]$ define the Sobolev space of order s on $\partial\Omega_\phi$ by

$$H^s(\partial\Omega_\phi) := \{h \in L^2(\partial\Omega_\phi) : x' \mapsto h(x', \phi(x')) \in H^s(\mathbb{R}^{n-1})\}$$

and equip $H^s(\partial\Omega_\phi)$ with the corresponding Hilbert space scalar product

$$(h, k)_{H^s(\partial\Omega_\phi)} := \big(h(\cdot, \phi(\cdot)), k(\cdot, \phi(\cdot))\big)_{H^s(\mathbb{R}^{n-1})}, \quad h, k \in H^s(\partial\Omega_\phi). \tag{8.2.6}$$

Note that the operator $V_\phi : H^s(\partial\Omega_\phi) \to H^s(\mathbb{R}^{n-1})$ that maps $h \in H^s(\partial\Omega_\phi)$ to the function $x' \mapsto h(x', \phi(x')) \in H^s(\mathbb{R}^{n-1})$ is an isometric isomorphism.

In the next step the notion of C^2-hypograph is replaced by a bounded domain with a C^2-smooth boundary, that is, the boundary is locally the boundary of a C^2-hypograph.

Definition 8.2.1. A bounded nonempty open subset $\Omega \subset \mathbb{R}^n$ is called a C^2-*domain* if there exist open sets $U_1, \dots, U_l \subset \mathbb{R}^n$ and (possibly up to rotations of coordinates) C^2-hypographs $\Omega_1, \dots, \Omega_l \subset \mathbb{R}^n$ such that

$$\partial\Omega \subset \bigcup_{j=1}^{l} U_j \quad \text{and} \quad \Omega \cap U_j = \Omega_j \cap U_j, \quad j = 1, \dots, l.$$

Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain as in Definition 8.2.1. Then the boundary $\partial\Omega \subset \mathbb{R}^n$ is compact and there exists a partition of unity subordinate to the open cover $\{U_j\}$ of $\partial\Omega$, that is, there exist functions $\eta_j \in C_0^\infty(\mathbb{R}^n)$, $j = 1, \dots, l$, with $\operatorname{supp}\eta_j \subset U_j$ such that $0 \le \eta_j(x) \le 1$ for all $x \in \mathbb{R}^n$ and $\sum_{j=1}^{l} \eta_j(x) = 1$ for all $x \in \partial\Omega$. For a measurable function $h : \partial\Omega \to \mathbb{C}$ the surface integral on $\partial\Omega$ is defined as

$$\int_{\partial\Omega} h \, d\sigma := \sum_{j=1}^{l} \int_{\mathbb{R}^{n-1}} \eta_j(x', \phi_j(x'))h(x', \phi_j(x'))\sqrt{1 + |\nabla\phi_j(x')|^2}\, dx',$$

where the C^2-functions $\phi_j : \mathbb{R}^{n-1} \to \mathbb{R}$ define the C^2-hypographs Ω_j as in (8.2.3) and the possible rotation of coordinates is suppressed. This surface integral induces a surface measure and the notion of an L^2-space $L^2(\partial\Omega)$ in the same way as in (8.2.4) and (8.2.5). In the present setting the Sobolev space $H^s(\partial\Omega)$ for $s \in [0, 2]$ is now defined by

$$H^s(\partial\Omega) := \bigl\{h \in L^2(\partial\Omega) : \eta_j h \in H^s(\partial\Omega_j),\, j = 1, \dots, l\bigr\}$$

and is equipped with the corresponding Hilbert space scalar product

$$(h, k)_{H^s(\partial\Omega)} = \sum_{j=1}^{l} (\eta_j h, \eta_j k)_{H^s(\partial\Omega_j)}, \quad h, k \in H^s(\partial\Omega). \tag{8.2.7}$$

It follows from the construction that $H^s(\partial\Omega)$ is densely and continuously embedded in $L^2(\partial\Omega)$ for $s \in [0, 2]$. Furthermore, since $\partial\Omega$ is a compact subset of $\mathbb{R}^n$, the embedding

$$H^t(\partial\Omega) \hookrightarrow H^s(\partial\Omega), \qquad 0 \le s < t \le 2, \tag{8.2.8}$$

is compact; see, e.g., [774, Theorem 7.10].

For later purposes it is convenient to use an equivalent characterization of the spaces $H^s(\partial\Omega)$ via interpolation; cf. [573, Theorem B.11]. More precisely, as in (8.1.6) it follows that there exists a unique uniformly positive self-adjoint operator Q in $L^2(\partial\Omega)$ such that

$$\operatorname{dom} Q = H^2(\partial\Omega) \quad \text{and} \quad (h, k)_{H^2(\partial\Omega)} = (Qh, Qk)_{L^2(\partial\Omega)} \tag{8.2.9}$$

for all $h, k \in H^2(\partial\Omega)$. It can be shown that the spaces $H^s(\partial\Omega)$ coincide with the domains $\operatorname{dom} Q^{s/2}$ for $s \in [0, 2]$ and that $(Q^{s/2}\cdot, Q^{s/2}\cdot)_{L^2(\partial\Omega)}$ defines a scalar product and equivalent norm in $H^s(\partial\Omega)$. The dual space of the antilinear continuous functionals on $H^s(\partial\Omega)$ is denoted by $H^{-s}(\partial\Omega)$, $s \in [0, 2]$. Then one obtains the following statement from Lemma 8.1.2 and Lemma 8.1.3.

Corollary 8.2.2. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain and let $s \in [0, 2]$. Then the following statements hold:*

(i) *$\{H^s(\partial\Omega), L^2(\partial\Omega), H^{-s}(\partial\Omega)\}$ is a Gelfand triple and the assertions in Lemma 8.1.2 hold with R, $\mathfrak{G}$, and $\mathfrak{G}'$ replaced by $Q^{s/2}$, $H^s(\partial\Omega)$, and $H^{-s}(\partial\Omega)$, respectively.*

(ii) *If* $\iota_+ : H^{1/2}(\partial\Omega) \to L^2(\partial\Omega)$ *and* $\iota_- : H^{-1/2}(\partial\Omega) \to L^2(\partial\Omega)$ *denote the isometric isomorphisms from Lemma* 8.1.2 (ii) *corresponding to the Gelfand triple* $\{H^{1/2}(\partial\Omega), L^2(\partial\Omega), H^{-1/2}(\partial\Omega)\}$ *such that*

$$(\iota_-\varphi, \iota_+\psi)_{L^2(\partial\Omega)} = \langle \varphi, \psi\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)}$$

holds for $\varphi \in H^{-1/2}(\partial\Omega)$ *and* $\psi \in H^{1/2}(\partial\Omega)$, *then for* $s \in [0, 3/2]$ *their restrictions*

$$\iota_+ = Q^{1/4} : H^{s+1/2}(\partial\Omega) \to H^s(\partial\Omega)$$

and

$$\iota_- = Q^{-1/4} : H^s(\partial\Omega) \to H^{s+1/2}(\partial\Omega)$$

are isometric isomorphisms such that $\iota_+\iota_-\phi = \phi$ *for* $\phi \in H^s(\partial\Omega)$ *and* $\iota_-\iota_+\chi = \chi$ *for* $\chi \in H^{s+1/2}(\partial\Omega)$*; here* Q *is the uniformly positive self-adjoint operator in* (8.2.9).

Assume now that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain as in Definition 8.2.1. The weak derivative of order $|\alpha|$ of an L^2-function f is denoted by $D^\alpha f$ in the following; as usual, here $\alpha \in \mathbb{N}_0^n$ stands for a multiindex and $|\alpha| = \alpha_1 + \cdots + \alpha_n$. Then for $k \in \mathbb{N}_0$ one has

$$H^k(\Omega) = \big\{ f \in L^2(\Omega) : D^\alpha f \in L^2(\Omega) \text{ for all } \alpha \in \mathbb{N}_0^n \text{ with } |\alpha| \le k \big\}$$

and

$$\|f\|_k := \sum_{|\alpha|\le k} \|D^\alpha f\|_{L^2(\Omega)}, \quad f \in H^k(\Omega), \tag{8.2.10}$$

is equivalent to the norm on $H^k(\Omega)$ in (8.2.1); cf. [573, Theorem 3.30]. Recall also that for $k \in \mathbb{N}$ there exists $C_k > 0$ such that the *Poincaré inequality*

$$\|f\|_k \le C_k \sum_{|\alpha|=k} \|D^\alpha f\|_{L^2(\Omega)}, \qquad f \in H_0^k(\Omega), \tag{8.2.11}$$

is valid. In particular, for $f \in C_0^\infty(\Omega)$ and $k = 2$, integration by parts and the Schwarz theorem give

$$\begin{aligned}\sum_{|\alpha|=2} \|D^\alpha f\|^2_{L^2(\Omega)} &= \sum_{|\alpha|=2} (D^\alpha f, D^\alpha f)_{L^2(\Omega)} \\ &= \sum_{j,k=1}^n (\partial_j\partial_k f, \partial_j\partial_k f)_{L^2(\Omega)} \\ &= \sum_{j,k=1}^n (\partial_j^2 f, \partial_k^2 f)_{L^2(\Omega)} \\ &= \|\Delta f\|^2_{L^2(\Omega)},\end{aligned}$$

and this equality extends to all $f \in H_0^2(\Omega)$ by (8.2.2). As a consequence one obtains the following useful fact.

Lemma 8.2.3. *The mapping $f \mapsto \|\Delta f\|_{L^2(\Omega)}$ is a norm on $H_0^2(\Omega)$ which is equivalent to the norms $\|\cdot\|_2$ and $\|\cdot\|_{H^2(\Omega)}$ in (8.2.10) and (8.2.1), respectively.*

Let again $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain and denote the unit normal vector field pointing outwards of $\partial\Omega$ by ν. The notion of *trace operator* or *trace map* and some of their properties are discussed next. Recall first that the mapping

$$C^\infty(\overline{\Omega}) \ni f \mapsto \left\{ f|_{\partial\Omega}, \frac{\partial f}{\partial \nu}\Big|_{\partial\Omega} \right\} \in H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)$$

extends by continuity to a continuous operator

$$H^2(\Omega) \ni f \mapsto \{\tau_{\mathrm{D}} f, \tau_{\mathrm{N}} f\} \in H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega), \tag{8.2.12}$$

which is surjective; here

$$\tau_{\mathrm{D}} : H^2(\Omega) \to H^{3/2}(\partial\Omega) \tag{8.2.13}$$

denotes the *Dirichlet trace operator* and

$$\tau_{\mathrm{N}} : H^2(\Omega) \to H^{1/2}(\partial\Omega) \tag{8.2.14}$$

denotes the *Neumann trace operator*. In particular, for all $f \in C^\infty(\overline{\Omega})$ one has

$$\tau_{\mathrm{D}} f = f|_{\Omega} \quad \text{and} \quad \tau_{\mathrm{N}} f = \frac{\partial f}{\partial \nu}|_{\partial\Omega},$$

respectively. With the help of the trace operators one has another useful characterization of the space $H_0^2(\Omega)$ in (8.2.2), namely,

$$H_0^2(\Omega) = \big\{ f \in H^2(\Omega) : \tau_{\mathrm{D}} f = \tau_{\mathrm{N}} f = 0 \big\}. \tag{8.2.15}$$

It will also be used that the Dirichlet trace operator $\tau_{\mathrm{D}} : H^2(\Omega) \to H^{3/2}(\partial\Omega)$ admits a continuous surjective extension

$$\tau_{\mathrm{D}}^{(1)} : H^1(\Omega) \to H^{1/2}(\partial\Omega), \tag{8.2.16}$$

which, in analogy to (8.2.15), leads to the characterization

$$H_0^1(\Omega) = \big\{ f \in H^1(\Omega) : \tau_{\mathrm{D}}^{(1)} f = 0 \big\}. \tag{8.2.17}$$

Recall next that for $f \in H^2(\Omega)$ and $g \in H^1(\Omega)$ the *first Green identity*

$$(-\Delta f, g)_{L^2(\Omega)} = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} - \big(\tau_{\mathrm{N}} f, \tau_{\mathrm{D}}^{(1)} g\big)_{L^2(\partial\Omega)} \tag{8.2.18}$$

holds. Note that $\tau_{\mathrm{N}} f, \tau_{\mathrm{D}} g \in H^{1/2}(\partial\Omega)$ by (8.2.14) and (8.2.16). If, in addition, also $g \in H^2(\Omega)$, then one concludes from (8.2.18) the second Green identity

$$(-\Delta f, g)_{L^2(\Omega)} - (f, -\Delta g)_{L^2(\Omega)} = (\tau_{\mathrm{D}} f, \tau_{\mathrm{N}} g)_{L^2(\partial\Omega)} - (\tau_{\mathrm{N}} f, \tau_{\mathrm{D}} g)_{L^2(\partial\Omega)}, \quad (8.2.19)$$

which is valid for all $f, g \in H^2(\Omega)$.

In the next lemma it will be shown that the Neumann trace operator τ_{N} in (8.2.14) admits an extension to the subspace of $H^1(\Omega)$ consisting of all those functions $f \in H^1(\Omega)$ such that $\Delta f \in L^2(\Omega)$, and it turns out that the first Green identity (8.2.18) remains valid in an extended form. Here, and in the following, the expression Δf is understood in the sense of distributions. If, in addition, one has that $\Delta f \in L^2(\Omega)$, then Δf is a regular distribution generated by the function $\Delta f \in L^2(\Omega)$ via

$$(\Delta f)(\varphi) = \int_\Omega (\Delta f)(x)\, \overline{\varphi(x)}\, dx, \qquad \varphi \in C_0^\infty(\Omega). \quad (8.2.20)$$

Lemma 8.2.4. *For $f \in H^1(\Omega)$ with $\Delta f \in L^2(\Omega)$ there exists a unique element $\varphi \in H^{-1/2}(\partial\Omega)$ such that*

$$(-\Delta f, g)_{L^2(\Omega)} = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} - \big\langle \varphi, \tau_{\mathrm{D}}^{(1)} g \big\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} \quad (8.2.21)$$

holds for all $g \in H^1(\Omega)$. In the following the notation $\tau_{\mathrm{N}}^{(1)} f := \varphi$ will be used.

Proof. Notice that there exists a bounded right inverse of $\tau_{\mathrm{D}}^{(1)}$ in (8.2.16), that is, there is a bounded operator $\eta : H^{1/2}(\partial\Omega) \to H^1(\Omega)$ with the property

$$\tau_{\mathrm{D}}^{(1)} \eta\psi = \psi, \qquad \psi \in H^{1/2}(\partial\Omega).$$

For a fixed $f \in H^1(\Omega)$ such that $\Delta f \in L^2(\Omega)$ define the antilinear functional $\varphi : H^{1/2}(\partial\Omega) \to \mathbb{C}$ by

$$\varphi(\psi) := (\nabla f, \nabla \eta\psi)_{L^2(\Omega;\mathbb{C}^n)} + (\Delta f, \eta\psi)_{L^2(\Omega)}, \quad \psi \in H^{1/2}(\partial\Omega). \quad (8.2.22)$$

Then one has

$$\begin{aligned} |\varphi(\psi)| &\le \|\nabla f\|_{L^2(\Omega;\mathbb{C}^n)} \|\nabla \eta\psi\|_{L^2(\Omega;\mathbb{C}^n)} + \|\Delta f\|_{L^2(\Omega)} \|\eta\psi\|_{L^2(\Omega)} \\ &\le C \|\eta\psi\|_{H^1(\Omega)} \\ &\le C' \|\psi\|_{H^{1/2}(\partial\Omega)} \end{aligned}$$

with some constants $C, C' > 0$, and hence $\varphi \in H^{-1/2}(\partial\Omega)$. Thus, (8.2.22) can also be written in the form

$$\langle \varphi, \psi \rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} = (\nabla f, \nabla \eta\psi)_{L^2(\Omega;\mathbb{C}^n)} + (\Delta f, \eta\psi)_{L^2(\Omega)}, \quad (8.2.23)$$

where $\psi \in H^{1/2}(\partial\Omega)$. Now let $g \in H^1(\Omega)$ and set $g_0 := g - \eta\tau_{\mathrm{D}}^{(1)} g$. Then it follows from the characterization of the space $H_0^1(\Omega)$ in (8.2.17) that $g_0 \in H_0^1(\Omega)$, and hence (8.2.2) shows that there is a sequence $(g_m) \subset C_0^\infty(\Omega)$ such that $g_m \to g_0$ in $H^1(\Omega)$. It follows that

$$\begin{aligned}(\nabla f, \nabla g_0)_{L^2(\Omega;\mathbb{C}^n)} &= \lim_{m\to\infty} (\nabla f, \nabla g_m)_{L^2(\Omega;\mathbb{C}^n)} \\ &= -\lim_{m\to\infty} (\Delta f, g_m)_{L^2(\Omega)} \\ &= -(\Delta f, g_0)_{L^2(\Omega)}\end{aligned}$$

and one obtains, together with (8.2.23) (and with $\psi = \tau_{\mathrm{D}}^{(1)} g$), that

$$\begin{aligned}(\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} &= \bigl(\nabla f, \nabla\bigl(g_0 + \eta\tau_{\mathrm{D}}^{(1)} g\bigr)\bigr)_{L^2(\Omega;\mathbb{C}^n)} \\ &= -(\Delta f, g_0)_{L^2(\Omega)} + \bigl(\nabla f, \nabla\bigl(\eta\tau_{\mathrm{D}}^{(1)} g\bigr)\bigr)_{L^2(\Omega;\mathbb{C}^n)} \\ &= -(\Delta f, g_0)_{L^2(\Omega)} + \bigl\langle \varphi, \tau_{\mathrm{D}}^{(1)} g\bigr\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} - \bigl(\Delta f, \eta\tau_{\mathrm{D}}^{(1)} g\bigr)_{L^2(\Omega)} \\ &= (-\Delta f, g)_{L^2(\Omega)} + \bigl\langle \varphi, \tau_{\mathrm{D}}^{(1)} g\bigr\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)}.\end{aligned}$$

This shows that $\varphi \in H^{-1/2}(\partial\Omega)$ in (8.2.22)–(8.2.23) satisfies (8.2.21).

It remains to check that $\varphi \in H^{-1/2}(\partial\Omega)$ in (8.2.21) is unique. Suppose that $\varphi_1, \varphi_2 \in H^{-1/2}(\partial\Omega)$ satisfy (8.2.21). Then

$$\bigl\langle \varphi_1 - \varphi_2, \tau_{\mathrm{D}}^{(1)} g\bigr\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} = 0$$

for all $g \in H^1(\Omega)$. As $\tau_{\mathrm{D}}^{(1)} : H^1(\Omega) \to H^{1/2}(\partial\Omega)$ is surjective it follows that $\varphi_1 - \varphi_2 = 0$ and hence φ in (8.2.21) is unique. □

Remark 8.2.5. The assertion in Lemma 8.2.4 and its proof extend in a natural manner to all $f \in H^1(\Omega)$ such that $-\Delta f \in H^1(\Omega)^*$. In this situation there still exists a unique element $\varphi \in H^{-1/2}(\partial\Omega)$ such that (instead of (8.2.21)) one has the slightly more general first Green identity

$$\langle -\Delta f, g\rangle_{H^1(\Omega)^*\times H^1(\Omega)} = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} - \bigl\langle \varphi, \tau_{\mathrm{D}}^{(1)} g\bigr\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)}$$

for all $g \in H^1(\Omega)$; cf. [573, Lemma 4.3].

8.3 Trace maps for the maximal Schrödinger operator

The differential expression $-\Delta + V$ is considered on a bounded domain Ω, where the function $V \in L^\infty(\Omega)$ is assumed to be real. One then associates with $-\Delta + V$ a preminimal, minimal and maximal operator in $L^2(\Omega)$, which are adjoints of each other. Furthermore, the Dirichlet and Neumann operators are defined via the corresponding sesquilinear form and the first representation theorem, and some of their properties are collected. In the case where Ω is a bounded C^2-domain it is shown in Theorem 8.3.9 and Theorem 8.3.10 that the Dirichlet and Neumann trace operators in the previous section admit continuous extensions to the maximal domain; this is a key ingredient in the construction of a boundary triplet in the next section.

Let $n \geq 2$, let $\Omega \subset \mathbb{R}^n$ be a bounded domain, and assume that the function $V \in L^\infty(\Omega)$ is real. The *preminimal operator* associated to the differential expression $-\Delta + V$ is defined as

$$T_0 = -\Delta + V, \qquad \operatorname{dom} T_0 = C_0^\infty(\Omega).$$

It follows immediately from

$$(T_0 f, f)_{L^2(\Omega)} = (\nabla f, \nabla f)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, f)_{L^2(\Omega)}, \quad f \in \operatorname{dom} T_0,$$

that T_0 is a densely defined symmetric operator in $L^2(\Omega)$ which is bounded from below with $v_- := \operatorname{essinf} V$ as a lower bound, so that $T_0 - v_-$ is nonnegative. Actually, for $f \in \operatorname{dom} T_0$ one has

$$\bigl((T_0 - v_-)f, f\bigr)_{L^2(\Omega)} = (\nabla f, \nabla f)_{L^2(\Omega;\mathbb{C}^n)} + \bigl((V - v_-)f, f\bigr)_{L^2(\Omega)} \geq \|\nabla f\|^2_{L^2(\Omega;\mathbb{C}^n)}$$

and hence, by the Poincaré inequality (8.2.11),

$$\bigl((T_0 - v_-)f, f\bigr)_{L^2(\Omega)} \geq C\|f\|_1^2 \geq C\|f\|^2_{L^2(\Omega)} \tag{8.3.1}$$

with some constant $C > 0$. This shows that $T_0 - v_-$ is uniformly positive.

The closure of T_0 in $L^2(\Omega)$ is the *minimal operator*

$$T_{\min} = -\Delta + V, \qquad \operatorname{dom} T_{\min} = H_0^2(\Omega). \tag{8.3.2}$$

In fact, using Lemma 8.2.3 and the fact that $V \in L^\infty(\Omega)$ one obtains that the graph norm

$$\|\cdot\|_{L^2(\Omega)} + \|T_{\min} \cdot\|_{L^2(\Omega)}$$

is equivalent to the H^2-norm on the closed subspace $H_0^2(\Omega)$ of $H^2(\Omega)$. Hence, $T_{\min}$ is a closed operator in $L^2(\Omega)$ and it follows from (8.2.2) that $\overline{T}_0 = T_{\min}$. Therefore, $T_{\min}$ is a densely defined closed symmetric operator in $L^2(\Omega)$ and $T_{\min} - v_-$ is uniformly positive.

Besides the preminimal and minimal operator, also the *maximal operator* $T_{\max}$ associated with $-\Delta + V$ in $L^2(\Omega)$ will be important in the sequel; it is defined by

$$\begin{aligned} T_{\max} &= -\Delta + V, \\ \operatorname{dom} T_{\max} &= \bigl\{ f \in L^2(\Omega) : -\Delta f + Vf \in L^2(\Omega) \bigr\}. \end{aligned} \tag{8.3.3}$$

Here the expression Δf for $f \in L^2(\Omega)$ is understood in the distributional sense. Since $V \in L^\infty(\Omega)$, it is clear that $f \in L^2(\Omega)$ belongs to $\operatorname{dom} T_{\max}$ if and only if $\Delta f \in L^2(\Omega)$, that is, the (regular) distribution Δf is generated by an L^2-function; cf. (8.2.20). Observe that $H^2(\Omega) \subset \operatorname{dom} T_{\max}$, and it will also turn out that $H^2(\Omega) \neq \operatorname{dom} T_{\max}$.

Proposition 8.3.1. *Let T_0, $T_{\min}$, and $T_{\max}$ be the preminimal, minimal, and maximal operator associated with $-\Delta + V$ in $L^2(\Omega)$, respectively. Then $\overline{T}_0 = T_{\min}$, and*

$$(T_{\min})^* = T_{\max} \quad \text{and} \quad T_{\min} = (T_{\max})^*. \tag{8.3.4}$$

Proof. It has already been shown above that $\overline{T}_0 = T_{\min}$ holds. In particular, this implies $T_0^* = (T_{\min})^*$ and thus for the first identity in (8.3.4) it suffices to show $T_0^* = T_{\max}$. Furthermore, since multiplication by $V \in L^\infty(\Omega)$ is a bounded operator in $L^2(\Omega)$, it is no restriction to assume $V = 0$ in the following. Let $f \in \operatorname{dom} T_0^*$ and consider $T_0^* f \in L^2(\Omega)$ as a distribution. Then one has for all $\varphi \in C_0^\infty(\Omega) = \operatorname{dom} T_0$

$$(T_0^* f)(\varphi) = (T_0^* f, \overline{\varphi})_{L^2(\Omega)} = (f, T_0\overline{\varphi})_{L^2(\Omega)} = (f, -\Delta\overline{\varphi})_{L^2(\Omega)} = (-\Delta f)(\varphi),$$

and hence $-\Delta f = T_0^* f \in L^2(\Omega)$. Thus, $f \in \operatorname{dom} T_{\max}$ and $T_{\max} f = T_0^* f$. Conversely, for $f \in \operatorname{dom} T_{\max}$ and all $\varphi \in C_0^\infty(\Omega) = \operatorname{dom} T_0$ one has

$$(T_0\varphi, f)_{L^2(\Omega)} = (-\Delta\varphi, f)_{L^2(\Omega)} = (\varphi, -\Delta f)_{L^2(\Omega)},$$

that is, $f \in \operatorname{dom} T_0^*$ and $T_0^* f = -\Delta f = T_{\max} f$. Thus, the first identity in (8.3.4) has been shown. The second identity in (8.3.4) follows by taking adjoints. □

In the following the self-adjoint *Dirichlet realization* A_D and the self-adjoint *Neumann realization* A_N of $-\Delta + V$ in $L^2(\Omega)$ will play an important role. The operators A_D and A_N will be introduced via the corresponding sesquilinear forms using the first representation theorem. More precisely, consider the densely defined forms

$$\mathfrak{t}_D[f, g] = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)}, \quad \operatorname{dom} \mathfrak{t}_D = H_0^1(\Omega),$$

and

$$\mathfrak{t}_N[f, g] = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)}, \quad \operatorname{dom} \mathfrak{t}_N = H^1(\Omega),$$

in $L^2(\Omega)$. It is easy to see that both forms are semibounded from below and that $v_- = \operatorname{essinf} V$ is a lower bound. The same argument as in (8.3.1) using the Poincaré inequality (8.2.11) on $\operatorname{dom} \mathfrak{t}_D = H_0^1(\Omega)$ implies the stronger statement that the form $\mathfrak{t}_D - v_-$ is uniformly positive. Furthermore, it follows from the definitions that the form $(\nabla\cdot, \nabla\cdot)_{L^2(\Omega;\mathbb{C}^n)}$ defined on $H_0^1(\Omega)$ or $H^1(\Omega)$ is closed in $L^2(\Omega)$; cf. Lemma 5.1.9. Since $V \in L^\infty(\Omega)$, it is clear that the form $(V\cdot, \cdot)_{L^2(\Omega)}$ is bounded on $L^2(\Omega)$ and hence it follows from Theorem 5.1.16 that also the forms $\mathfrak{t}_D$ and $\mathfrak{t}_N$ are closed in $L^2(\Omega)$. Therefore, by the first representation theorem (Theorem 5.1.18), there exist unique semibounded self-adjoint operators A_D and A_N in $L^2(\Omega)$ associated with $\mathfrak{t}_D$ and $\mathfrak{t}_N$, respectively, such that

$$(A_D f, g)_{L^2(\Omega)} = \mathfrak{t}_D[f, g] \quad \text{for } f \in \operatorname{dom} A_D,\ g \in \operatorname{dom} \mathfrak{t}_D,$$

and

$$(A_N f, g)_{L^2(\Omega)} = \mathfrak{t}_N[f, g] \quad \text{for } f \in \operatorname{dom} A_N,\ g \in \operatorname{dom} \mathfrak{t}_N.$$

The self-adjoint operators $A_{\rm D}$ and $A_{\rm N}$ are called the *Dirichlet operator* and *Neumann operator*, respectively. In the next propositions some properties of these operators are discussed.

Proposition 8.3.2. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded domain. Then the Dirichlet operator $A_{\rm D}$ is given by*

$$\begin{aligned} A_{\rm D} f &= -\Delta f + Vf, \\ \operatorname{dom} A_{\rm D} &= \bigl\{ f \in H_0^1(\Omega) : -\Delta f + Vf \in L^2(\Omega) \bigr\}, \end{aligned} \tag{8.3.5}$$

and for all $\lambda \in \rho(A_{\rm D})$ the resolvent $(A_{\rm D}-\lambda)^{-1}$ is a compact operator in $L^2(\Omega)$. The Dirichlet operator $A_{\rm D}$ coincides with the Friedrichs extension $S_{\rm F}$ of the minimal operator $T_{\min}$ in (8.3.2). In particular, $A_{\rm D}-v_-$ is uniformly positive. Furthermore, if $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain, then the Dirichlet operator $A_{\rm D}$ is given by

$$\begin{aligned} A_{\rm D} f &= -\Delta f + Vf, \\ \operatorname{dom} A_{\rm D} &= \bigl\{ f \in H^1(\Omega) : -\Delta f + Vf \in L^2(\Omega),\, \tau_{\rm D}^{(1)} f = 0 \bigr\}. \end{aligned} \tag{8.3.6}$$

Proof. Observe that for $f \in \operatorname{dom} A_{\rm D}$ and $g \in C_0^\infty(\Omega) \subset \operatorname{dom} \mathfrak{t}_{\rm D}$ one has

$$(A_{\rm D} f, g)_{L^2(\Omega)} = \mathfrak{t}_{\rm D}[f,g] = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)} = \bigl(-\Delta f + Vf\bigr)(\bar g),$$

where $-\Delta f + Vf$ is viewed as a distribution. Since this identity holds for all $g \in C_0^\infty(\Omega)$ and $A_{\rm D}$ is an operator in $L^2(\Omega)$ it follows that

$$-\Delta f + Vf = A_{\rm D} f \in L^2(\Omega).$$

Therefore, $A_{\rm D}$ is given by (8.3.5). In the case that $\Omega \subset \mathbb{R}^n$ has a C^2-smooth boundary the form of the domain of $A_{\rm D}$ in (8.3.6) follows from (8.3.5) and (8.2.17).

Next it will be shown that for $\lambda \in \rho(A_{\rm D})$ the resolvent $(A_{\rm D} - \lambda)^{-1}$ is a compact operator in $L^2(\Omega)$. For this observe first that

$$(A_{\rm D} - \lambda)^{-1} : L^2(\Omega) \to H_0^1(\Omega), \quad \lambda \in \rho(A_{\rm D}), \tag{8.3.7}$$

is everywhere defined and closed as an operator from $L^2(\Omega)$ into $H_0^1(\Omega)$. In fact, if $f_n \to f$ in $L^2(\Omega)$ and $(A_{\rm D} - \lambda)^{-1} f_n \to h$ in $H_0^1(\Omega)$, then $(A_{\rm D} - \lambda)^{-1} f_n \to h$ in $L^2(\Omega)$, and since the operator $(A_{\rm D} - \lambda)^{-1}$ is everywhere defined and continuous in $L^2(\Omega)$, it is clear that $(A_{\rm D} - \lambda)^{-1} f = h$. Hence, the operator in (8.3.7) is bounded by the closed graph theorem. By Rellich's theorem the embedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ is compact, and it follows that $(A_{\rm D} - \lambda)^{-1}$, $\lambda \in \rho(A_{\rm D})$, is a compact operator in $L^2(\Omega)$.

It remains to verify that $A_{\rm D}$ is the Friedrichs extension $S_{\rm F}$ of $T_{\min} = \overline{T}_0$ or, equivalenty, the Friedrichs extension of T_0; cf. Lemma 5.3.1 and Definition 5.3.2. For this, consider the form $\mathfrak{t}_{T_0}[f,g] = (T_0 f, g)_{L^2(\Omega)}$, defined for $f, g \in \operatorname{dom} T_0$, and note that

$$\mathfrak{t}_{T_0}[f,g] = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)}, \quad \operatorname{dom} \mathfrak{t}_{T_0} = C_0^\infty(\Omega).$$

Observe that $f_m \to_{\mathfrak{t}_{T_0}} f$ if and only if $f_m \to f$ in $L^2(\Omega)$ and (∇f_m) is a Cauchy sequence in $L^2(\Omega; \mathbb{C}^n)$. Hence, $f_m \to_{\mathfrak{t}_{T_0}} f$ implies $f_m \to f$ in the norm of $H^1(\Omega)$, and so $f \in H_0^1(\Omega)$ by (8.2.2). Therefore, by (5.1.16), the closure of the form $\mathfrak{t}_{T_0}$ is given by

$$\widetilde{\mathfrak{t}}_{T_0}[f,g] = \lim_{m\to\infty} \mathfrak{t}_{T_0}[f_m, g_m] = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)},$$

where $f, g \in H_0^1(\Omega)$ and $f_m \to_{\mathfrak{t}_{T_0}} f$, $g_m \to_{\mathfrak{t}_{T_0}} g$. Hence, $\widetilde{\mathfrak{t}}_{T_0} = \mathfrak{t}_{\mathrm{D}}$, and since by Definition 5.3.2 the Friedrichs extension of T_0 is the unique self-adjoint operator corresponding to the closed form $\widetilde{\mathfrak{t}}_{T_0}$, the assertion follows. □

In order to specify the Neumann operator A_{N}, the first Green identity and the trace operators $\tau_{\mathrm{D}}^{(1)} : H^1(\Omega) \to H^{1/2}(\partial\Omega)$ and $\tau_{\mathrm{N}}^{(1)} : H^1(\Omega) \to H^{-1/2}(\partial\Omega)$ will be used; cf. Lemma 8.2.4. For this reason in the next proposition it is assumed that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain. It is also important to note that the Neumann operator A_{N} below differs from the Kreĭn–von Neumann extension and the Kreĭn type extensions in Definition 5.4.2; cf. Section 8.5 for more details.

Proposition 8.3.3. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain. Then the Neumann operator A_{N} is given by*

$$\begin{aligned} A_{\mathrm{N}} f &= -\Delta f + Vf, \\ \operatorname{dom} A_{\mathrm{N}} &= \bigl\{ f \in H^1(\Omega) : -\Delta f + Vf \in L^2(\Omega),\ \tau_{\mathrm{N}}^{(1)} f = 0 \bigr\}, \end{aligned} \tag{8.3.8}$$

and for all $\lambda \in \rho(A_{\mathrm{N}})$ the resolvent $(A_{\mathrm{N}} - \lambda)^{-1}$ is a compact operator in $L^2(\Omega)$.

Proof. In a first step it follows for $f \in \operatorname{dom} A_{\mathrm{N}} \subset H^1(\Omega)$ and all $g \in C_0^\infty(\Omega)$ in the same way as in the proof of Proposition 8.3.2 that

$$(A_{\mathrm{N}} f, g)_{L^2(\Omega)} = \mathfrak{t}_{\mathrm{N}}[f,g] = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)} = \bigl(-\Delta f + Vf\bigr)(\bar{g}),$$

and hence $A_{\mathrm{N}} f = (-\Delta + V) f \in L^2(\Omega)$. In particular, for $f \in \operatorname{dom} A_{\mathrm{N}}$ one has $f \in H^1(\Omega)$ and $-\Delta f \in L^2(\Omega)$, so that Lemma 8.2.4 applies and yields

$$\begin{aligned} (A_{\mathrm{N}} f, g)_{L^2(\Omega)} &= \mathfrak{t}_{\mathrm{N}}[f,g] \\ &= (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} + (Vf, g)_{L^2(\Omega)} \\ &= \bigl((-\Delta + V)f, g\bigr)_{L^2(\Omega)} + \bigl\langle \tau_{\mathrm{N}}^{(1)} f, \tau_{\mathrm{D}}^{(1)} g \bigr\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} \end{aligned}$$

for all $g \in \operatorname{dom} \mathfrak{t}_{\mathrm{N}} = H^1(\Omega)$. As $A_{\mathrm{N}} f = (-\Delta + V) f$, one concludes that

$$\bigl\langle \tau_{\mathrm{N}}^{(1)} f, \tau_{\mathrm{D}}^{(1)} g \bigr\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} = 0 \quad \text{for all } g \in H^1(\Omega).$$

Since $\tau_{\mathrm{D}}^{(1)} : H^1(\Omega) \to H^{1/2}(\partial\Omega)$ is surjective, it follows that $\tau_{\mathrm{N}}^{(1)} f = 0$. This implies the representation (8.3.8).

To show that the resolvent $(A_{\mathrm{N}} - \lambda)^{-1}$ is a compact operator in $L^2(\Omega)$ one argues in the same way as in the proof of Proposition 8.3.2. In fact, the operator

$$(A_{\mathrm{N}} - \lambda)^{-1} : L^2(\Omega) \to H^1(\Omega), \quad \lambda \in \rho(A_{\mathrm{N}}),$$

is everywhere defined and closed, and hence bounded by the closed graph theorem. Since $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain, the embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$ is compact and this implies that $(A_{\mathrm{N}} - \lambda)^{-1}$, $\lambda \in \rho(A_{\mathrm{N}})$, is a compact operator in $L^2(\Omega)$. □

It is known that functions f in $\operatorname{dom} A_{\mathrm{D}}$ or $\operatorname{dom} A_{\mathrm{N}}$ are locally H^2-regular, that is, for every compact subset $K \subset \Omega$ the restriction of f to K is in $H^2(K)$. The next theorem is an important elliptic regularity result which ensures H^2-regularity of the functions in $\operatorname{dom} A_{\mathrm{D}}$ or $\operatorname{dom} A_{\mathrm{N}}$ in (8.3.6) and (8.3.8), respectively, up to the boundary if the bounded domain Ω is C^2-smooth in the sense of Definition 8.2.1.

Theorem 8.3.4. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain. Then one has*

$$A_{\mathrm{D}} f = -\Delta f + V f, \quad \operatorname{dom} A_{\mathrm{D}} = \bigl\{ f \in H^2(\Omega) : \tau_{\mathrm{D}} f = 0 \bigr\},$$

and

$$A_{\mathrm{N}} f = -\Delta f + V f, \quad \operatorname{dom} A_{\mathrm{N}} = \bigl\{ f \in H^2(\Omega) : \tau_{\mathrm{N}} f = 0 \bigr\}.$$

Note that under the assumptions in Theorem 8.3.4 the domain of the Dirichlet operator A_{D} is $H^2(\Omega) \cap H^1_0(\Omega)$; cf. (8.2.17). The direct sum decompositions in the next corollary follow immediately from Theorem 1.7.1 when considering the operator $T = -\Delta + V$, $\operatorname{dom} T = H^2(\Omega)$, and taking into account that $A_{\mathrm{D}} \subset T$ and $A_{\mathrm{N}} \subset T$.

Corollary 8.3.5. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain and denote by $\tau_{\mathrm{D}} : H^2(\Omega) \to H^{3/2}(\partial\Omega)$ and $\tau_{\mathrm{N}} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$ the Dirichlet and Neumann trace operator in (8.2.13) and (8.2.14), respectively. Then for $\lambda \in \rho(A_{\mathrm{D}})$ one has the direct sum decomposition*

$$\begin{aligned} H^2(\Omega) &= \operatorname{dom} A_{\mathrm{D}} \dotplus \bigl\{ f_\lambda \in H^2(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\} \\ &= \ker \tau_{\mathrm{D}} \dotplus \bigl\{ f_\lambda \in H^2(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\}, \end{aligned} \tag{8.3.9}$$

and for $\lambda \in \rho(A_{\mathrm{N}})$ one has the direct sum decomposition

$$\begin{aligned} H^2(\Omega) &= \operatorname{dom} A_{\mathrm{N}} \dotplus \bigl\{ f_\lambda \in H^2(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\} \\ &= \ker \tau_{\mathrm{N}} \dotplus \bigl\{ f_\lambda \in H^2(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\}. \end{aligned} \tag{8.3.10}$$

As a consequence of the decomposition (8.3.9) in Corollary 8.3.5 and (8.2.12) one concludes that the so-called Dirichlet-to-Neumann map in the next definition is a well-defined operator from $H^{3/2}(\partial\Omega)$ into $H^{1/2}(\partial\Omega)$.

Definition 8.3.6. Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let A_{D} be the self-adjoint Dirichlet operator, and let $\tau_{\mathrm{D}} : H^2(\Omega) \to H^{3/2}(\partial\Omega)$ and $\tau_{\mathrm{N}} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$

be the Dirichlet and Neumann trace operator in (8.2.13) and (8.2.14), respectively. For $\lambda \in \rho(A_{\mathrm{D}})$ the *Dirichlet-to-Neumann map* is defined as

$$D(\lambda) : H^{3/2}(\partial\Omega) \to H^{1/2}(\partial\Omega), \qquad \tau_{\mathrm{D}} f_\lambda \mapsto \tau_{\mathrm{N}} f_\lambda,$$

where $f_\lambda \in H^2(\Omega)$ is such that $(-\Delta + V) f_\lambda = \lambda f_\lambda$.

Note that for $\lambda \in \rho(A_{\mathrm{D}}) \cap \rho(A_{\mathrm{N}})$ both decompositions (8.3.9) and (8.3.10) in Corollary 8.3.5 hold and together with (8.2.12) this implies that the Dirichlet-to-Neumann map $D(\lambda)$ is a bijective operator from $H^{3/2}(\partial\Omega)$ onto $H^{1/2}(\partial\Omega)$.

A further useful consequence of Theorem 8.3.4 is given by the following a priori estimates.

Corollary 8.3.7. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain and let A_{D} and A_{N} be the Dirichlet and Neumann operator, respectively. Then there exist constants $C_{\mathrm{D}} > 0$ and $C_{\mathrm{N}} > 0$ such that*

$$\|f\|_{H^2(\Omega)} \le C_{\mathrm{D}} \big(\|f\|_{L^2(\Omega)} + \|A_{\mathrm{D}} f\|_{L^2(\Omega)} \big), \quad f \in \operatorname{dom} A_{\mathrm{D}},$$

and

$$\|g\|_{H^2(\Omega)} \le C_{\mathrm{N}} \big(\|g\|_{L^2(\Omega)} + \|A_{\mathrm{N}} g\|_{L^2(\Omega)} \big), \quad g \in \operatorname{dom} A_{\mathrm{N}}.$$

Proof. One verifies in the same way as in the proof of Proposition 8.3.2 that for $\lambda \in \rho(A_{\mathrm{D}})$ the operator $(A_{\mathrm{D}} - \lambda)^{-1} : L^2(\Omega) \to H^2(\Omega)$ is everywhere defined and closed, and hence bounded. For $f \in \operatorname{dom} A_{\mathrm{D}}$ choose $h \in L^2(\Omega)$ such that $f = (A_{\mathrm{D}} - \lambda)^{-1} h$. Then

$$\|f\|_{H^2(\Omega)} = \|(A_{\mathrm{D}} - \lambda)^{-1} h\|_{H^2(\Omega)} \le C \|h\|_{L^2(\Omega)} = C_{\mathrm{D}} \|(A_{\mathrm{D}} - \lambda) f\|_{L^2(\Omega)}$$

for some $C > 0$ and $C_{\mathrm{D}} > 0$, and the first estimate follows. The second estimate is proved in the same way. ☐

The next lemma is an important ingredient in the following.

Lemma 8.3.8. *Let $T_{\max}$ be the maximal operator associated to $-\Delta + V$ in (8.3.3). Then the space $C^\infty(\overline{\Omega})$ is dense in $\operatorname{dom} T_{\max}$ with respect to the graph norm.*

Proof. Since $V \in L^\infty(\Omega)$ is bounded, the graph norms

$$\big(\|\cdot\|^2_{L^2(\Omega)} + \|T_{\max} \cdot\|^2_{L^2(\Omega)} \big)^{1/2} \quad \text{and} \quad \big(\|\cdot\|^2_{L^2(\Omega)} + \|\Delta \cdot\|^2_{L^2(\Omega)} \big)^{1/2}$$

are equivalent on $\operatorname{dom} T_{\max}$, and hence it is no restriction to assume that $V = 0$. Now suppose that $f \in \operatorname{dom} T_{\max}$ is such that for all $g \in C^\infty(\overline{\Omega})$

$$0 = (f, g)_{L^2(\Omega)} + (\Delta f, \Delta g)_{L^2(\Omega)}. \tag{8.3.11}$$

Then (8.3.11) holds for all $g \in C_0^\infty(\Omega)$, so that $0 = (f + \Delta^2 f)(\bar{g})$, where $f + \Delta^2 f$ is viewed as a distribution. As $f \in L^2(\Omega)$, one concludes that

$$\Delta^2 f = -f \in L^2(\Omega). \tag{8.3.12}$$

Next it will be shown that

$$\Delta f \in H_0^2(\Omega). \tag{8.3.13}$$

In fact, choose an open ball B such that $\overline{\Omega} \subset B$ and let $h \in C_0^\infty(B)$. Let

$$\widetilde{A}_{\rm D} = -\Delta, \qquad \operatorname{dom} \widetilde{A}_{\rm D} = H^2(B) \cap H_0^1(B),$$

be the self-adjoint Dirichlet Laplacian in $L^2(B)$; cf. Theorem 8.3.4. Since B is bounded, one has $0 \in \rho(\widetilde{A}_{\rm D})$ by Proposition 8.3.2. As $h \in C_0^\infty(B)$, elliptic regularity yields $\widetilde{A}_{\rm D}^{-1} h \in C^\infty(B)$ and hence $(\widetilde{A}_{\rm D}^{-1} h)|_\Omega \in C^\infty(\overline{\Omega})$ for the restriction onto Ω. Denote by $\widetilde{f}$ and $\widetilde{\Delta f}$ the extension of f and Δf by zero to B. Then it follows with the help of (8.3.11) that

$$\begin{aligned}
(\widetilde{A}_{\rm D}^{-1} \widetilde{f}, h)_{L^2(B)} &= (\widetilde{f}, \widetilde{A}_{\rm D}^{-1} h)_{L^2(B)} \\
&= \bigl(f, (\widetilde{A}_{\rm D}^{-1} h)|_\Omega\bigr)_{L^2(\Omega)} \\
&= -\bigl(\Delta f, \Delta(\widetilde{A}_{\rm D}^{-1} h)|_\Omega\bigr)_{L^2(\Omega)} \\
&= (-\widetilde{\Delta f}, h)_{L^2(B)}
\end{aligned}$$

holds for $h \in C_0^\infty(B)$. This yields $-\widetilde{\Delta f} = \widetilde{A}_{\rm D}^{-1} \widetilde{f} \in H^2(B)$. Moreover, as $\widetilde{\Delta f}$ vanishes outside of Ω it follows that $\Delta f \in H_0^2(\Omega)$, that is, (8.3.13) holds.

Now choose a sequence $(\psi_k) \subset C_0^\infty(\Omega)$ such that $\psi_k \to \Delta f$ in $H^2(\Omega)$. Then, by (8.3.12),

$$\begin{aligned}
0 \leq (\Delta f, \Delta f)_{L^2(\Omega)} &= \lim_{k\to\infty} (\psi_k, \Delta f)_{L^2(\Omega)} = \lim_{k\to\infty} (\Delta \psi_k, f)_{L^2(\Omega)} \\
&= (\Delta^2 f, f)_{L^2(\Omega)} = -(f, f)_{L^2(\Omega)} \leq 0,
\end{aligned}$$

that is, $f = 0$ in (8.3.11). Hence, $C^\infty(\overline{\Omega})$ is dense in $\operatorname{dom} T_{\max}$ with respect to the graph norm. □

The following result on the extension of the Dirichlet trace operator onto $\operatorname{dom} T_{\max}$ is essential for the construction of a boundary triplet for $T_{\max}$.

Theorem 8.3.9. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain. Then the Dirichlet trace operator $\tau_{\rm D} : H^2(\Omega) \to H^{3/2}(\partial\Omega)$ in (8.2.13) admits a unique extension to a continuous surjective operator*

$$\widetilde{\tau}_{\rm D} : \operatorname{dom} T_{\max} \to H^{-1/2}(\partial\Omega),$$

where $\operatorname{dom} T_{\max}$ *is equipped with the graph norm. Furthermore,*

$$\ker \widetilde{\tau}_{\rm D} = \ker \tau_{\rm D} = \operatorname{dom} A_{\rm D}.$$

Proof. In the following fix $\lambda \in \rho(A_{\rm D})$ and consider the operator

$$\Upsilon := -\tau_{\rm N}(A_{\rm D} - \overline{\lambda})^{-1} : L^2(\Omega) \to H^{1/2}(\partial\Omega). \tag{8.3.14}$$

Since $(A_D - \bar{\lambda})^{-1} : L^2(\Omega) \to H^2(\Omega)$ is everywhere defined and closed, it is clear that $(A_D - \bar{\lambda})^{-1} : L^2(\Omega) \to H^2(\Omega)$ is continuous and maps onto $\operatorname{dom} A_D$. Hence, it follows from Theorem 8.3.4 and (8.2.12) that $\Upsilon \in \mathbf{B}(L^2(\Omega), H^{1/2}(\partial\Omega))$ in (8.3.14) is a surjective operator.

Next it will be shown that

$$\ker \Upsilon = \mathfrak{N}_\lambda(T_{\max})^\perp, \tag{8.3.15}$$

where $\mathfrak{N}_\lambda(T_{\max}) = \ker(T_{\max} - \lambda)$. In fact, for the inclusion $(\subset)$ in (8.3.15), assume that

$$\Upsilon h = -\tau_N(A_D - \bar{\lambda})^{-1} h = 0$$

for some $h \in L^2(\Omega)$. Then it follows from Theorem 8.3.4 that

$$(A_D - \bar{\lambda})^{-1} h \in \operatorname{dom} A_D \cap \operatorname{dom} A_N$$

and hence $(A_D - \bar{\lambda})^{-1} h \in \operatorname{dom} T_{\min}$ by (8.2.15) and (8.3.2). For $f_\lambda \in \mathfrak{N}_\lambda(T_{\max})$ one concludes, together with Proposition 8.3.1, that

$$\begin{aligned}(f_\lambda, h)_{L^2(\Omega)} &= \bigl(f_\lambda, (T_{\min} - \bar{\lambda})(A_D - \bar{\lambda})^{-1} h\bigr)_{L^2(\Omega)} \\ &= \bigl((T_{\max} - \lambda) f_\lambda, (A_D - \bar{\lambda})^{-1} h\bigr)_{L^2(\Omega)} \\ &= 0,\end{aligned}$$

which shows $h \in \mathfrak{N}_\lambda(T_{\max})^\perp$. For the inclusion $(\supset)$ in (8.3.15), let $h \in \mathfrak{N}_\lambda(T_{\max})^\perp$. Then $h \in \operatorname{ran}(T_{\min} - \bar{\lambda})$, and hence there exists $k \in \operatorname{dom} T_{\min} = H^2_0(\Omega)$ such that $h = (T_{\min} - \bar{\lambda})k$. It follows that

$$\Upsilon h = -\tau_N(A_D - \bar{\lambda})^{-1} h = -\tau_N(A_D - \bar{\lambda})^{-1}(T_{\min} - \bar{\lambda})k = -\tau_N k = 0,$$

which shows that $h \in \ker \Upsilon$. This completes the proof of (8.3.15).

From (8.3.14) and (8.3.15) it follows that the restriction of Υ to $\mathfrak{N}_\lambda(T_{\max})$ is an isomorphism from $\mathfrak{N}_\lambda(T_{\max})$ onto $H^{1/2}(\partial\Omega)$. This implies that the dual operator

$$\Upsilon' : H^{-1/2}(\partial\Omega) \to L^2(\Omega) \tag{8.3.16}$$

is bounded and invertible, and by the closed range theorem (see Theorem 1.3.5 for the Hilbert space adjoint) one has

$$\operatorname{ran} \Upsilon' = (\ker \Upsilon)^\perp = \mathfrak{N}_\lambda(T_{\max}).$$

The inverse $(\Upsilon')^{-1}$ is regarded as an isomorphism from $\mathfrak{N}_\lambda(T_{\max})$ onto $H^{-1/2}(\partial\Omega)$. Now recall the direct sum decomposition

$$\operatorname{dom} T_{\max} = \operatorname{dom} A_D \dotplus \mathfrak{N}_\lambda(T_{\max})$$

from Theorem 1.7.1 or Corollary 1.7.5, and write the elements $f \in \operatorname{dom} T_{\max}$ accordingly,

$$f = f_D + f_\lambda, \quad f_D \in \operatorname{dom} A_D, \quad f_\lambda \in \mathfrak{N}_\lambda(T_{\max}).$$

Define the mapping

$$\widetilde{\tau}_{\mathrm{D}} : \operatorname{dom} T_{\max} \to H^{-1/2}(\partial\Omega), \qquad f \mapsto \widetilde{\tau}_{\mathrm{D}} f = (\Upsilon')^{-1} f_\lambda. \tag{8.3.17}$$

Next it will be shown that $\widetilde{\tau}_{\mathrm{D}}$ is an extension of the Dirichlet trace operator $\tau_{\mathrm{D}} : H^2(\Omega) \to H^{3/2}(\partial\Omega)$. For this, consider $\varphi \in \operatorname{ran} \tau_{\mathrm{D}} = H^{3/2}(\partial\Omega) \subset H^{-1/2}(\partial\Omega)$ and note that by (8.3.9) and (8.2.12) there exists a unique $f_\lambda \in H^2(\Omega)$ such that

$$(-\Delta + V) f_\lambda = \lambda f_\lambda \quad \text{and} \quad \tau_{\mathrm{D}} f_\lambda = \varphi. \tag{8.3.18}$$

Let $h \in L^2(\Omega)$ and set $k := (A_{\mathrm{D}} - \bar{\lambda})^{-1} h$. Then, by (8.3.14), the fact that $\tau_{\mathrm{D}} k = 0$, and the second Green identity (8.2.19),

$$\begin{aligned}
(\Upsilon'\varphi, h)_{L^2(\Omega)} &= \langle \varphi, \Upsilon h \rangle_{H^{-1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)} \\
&= (\varphi, \Upsilon h)_{L^2(\partial\Omega)} \\
&= -\big(\varphi, \tau_{\mathrm{N}}(A_{\mathrm{D}} - \bar{\lambda})^{-1} h\big)_{L^2(\partial\Omega)} \\
&= -(\tau_{\mathrm{D}} f_\lambda, \tau_{\mathrm{N}} k)_{L^2(\partial\Omega)} + (\tau_{\mathrm{N}} f_\lambda, \tau_{\mathrm{D}} k)_{L^2(\partial\Omega)} \\
&= -\big((-\Delta + V) f_\lambda, k\big)_{L^2(\Omega)} + \big(f_\lambda, (-\Delta + V) k\big)_{L^2(\Omega)} \\
&= -(\lambda f_\lambda, k)_{L^2(\Omega)} + (f_\lambda, A_{\mathrm{D}} k)_{L^2(\Omega)} \\
&= \big(f_\lambda, (A_{\mathrm{D}} - \bar{\lambda}) k\big)_{L^2(\Omega)} \\
&= (f_\lambda, h)_{L^2(\Omega)},
\end{aligned}$$

and thus $\Upsilon'\varphi = f_\lambda$. Hence, the restriction of Υ' to $H^{3/2}(\partial\Omega)$ maps $\varphi \in H^{3/2}(\partial\Omega)$ to the unique $H^2(\Omega)$-solution f_λ of the boundary value problem (8.3.18), that is, to the unique element $f_\lambda \in \mathfrak{N}_\lambda(T_{\max}) \cap H^2(\Omega)$ such that $\tau_{\mathrm{D}} f_\lambda = \varphi$. Therefore, $(\Upsilon')^{-1}$ maps the elements in $\mathfrak{N}_\lambda(T_{\max}) \cap H^2(\Omega)$ onto their Dirichlet boundary values, that is,

$$(\Upsilon')^{-1} f_\lambda = \tau_{\mathrm{D}} f_\lambda \quad \text{for} \quad f_\lambda \in \mathfrak{N}_\lambda(T_{\max}) \cap H^2(\Omega).$$

By definition $\widetilde{\tau}_{\mathrm{D}} f_{\mathrm{D}} = 0 = \tau_{\mathrm{D}} f_{\mathrm{D}}$ for $f_{\mathrm{D}} \in \operatorname{dom} A_{\mathrm{D}}$. Therefore, if $f \in H^2(\Omega)$ is decomposed according to (8.3.9) as

$$f = f_{\mathrm{D}} + f_\lambda, \quad f_{\mathrm{D}} \in \operatorname{dom} A_{\mathrm{D}}, \quad f_\lambda \in \mathfrak{N}_\lambda(T_{\max}) \cap H^2(\Omega),$$

then

$$\widetilde{\tau}_{\mathrm{D}} f = \widetilde{\tau}_{\mathrm{D}}(f_{\mathrm{D}} + f_\lambda) = (\Upsilon')^{-1} f_\lambda = \tau_{\mathrm{D}} f_\lambda = \tau_{\mathrm{D}} f,$$

so that $\widetilde{\tau}_{\mathrm{D}}$ in (8.3.17) is an extension of τ_{D}. Note that by construction $\widetilde{\tau}_{\mathrm{D}}$ is surjective. Furthermore, the property $\ker \widetilde{\tau}_{\mathrm{D}} = \ker \tau_{\mathrm{D}}$ is clear from the definition.

It remains to show that $\widetilde{\tau}_{\mathrm{D}}$ in (8.3.17) is continuous with respect to the graph norm on $\operatorname{dom} T_{\max}$. For this, consider $f = f_{\mathrm{D}} + f_\lambda \in \operatorname{dom} T_{\max}$ with $f_{\mathrm{D}} \in \operatorname{dom} A_{\mathrm{D}}$ and $f_\lambda \in \mathfrak{N}_\lambda(T_{\max})$, and note that

$$\begin{aligned}
f_\lambda = f - f_{\mathrm{D}} &= f - (A_{\mathrm{D}} - \lambda)^{-1}(T_{\max} - \lambda) f_{\mathrm{D}} \\
&= f - (A_{\mathrm{D}} - \lambda)^{-1}(T_{\max} - \lambda) f.
\end{aligned}$$

Since $(\Upsilon')^{-1} : \mathfrak{N}_\lambda(T_{\max}) \to H^{-1/2}(\partial\Omega)$ is an isomorphism and hence, in particular, bounded, one has

$$\begin{aligned}\|\widetilde{\tau}_{\mathrm{D}} f\|_{H^{-1/2}(\partial\Omega)} &= \|(\Upsilon')^{-1} f_\lambda\|_{H^{-1/2}(\partial\Omega)} \\ &\le C\|f_\lambda\|_{L^2(\Omega)} \\ &\le C\big(\|f\|_{L^2(\Omega)} + \|(A_{\mathrm{D}} - \lambda)^{-1}(T_{\max} - \lambda)f\|_{L^2(\Omega)}\big) \\ &\le C'\big(\|f\|_{L^2(\Omega)} + \|(T_{\max} - \lambda)f\|_{L^2(\Omega)}\big) \\ &\le C''\big(\|f\|_{L^2(\Omega)} + \|T_{\max} f\|_{L^2(\Omega)}\big)\end{aligned}$$

with some constants $C, C', C'' > 0$. Thus, $\widetilde{\tau}_{\mathrm{D}}$ is continuous. The proof of Theorem 8.3.9 is complete. □

The following result is parallel to Theorem 8.3.9 and can be proved in a similar way.

Theorem 8.3.10. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain. Then the Neumann trace operator $\tau_{\mathrm{N}} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$ in (8.2.14) admits a unique extension to a continuous surjective operator*

$$\widetilde{\tau}_{\mathrm{N}} : \operatorname{dom} T_{\max} \to H^{-3/2}(\partial\Omega),$$

where $\operatorname{dom} T_{\max}$ *is equipped with the graph norm. Furthermore,*

$$\ker \widetilde{\tau}_{\mathrm{N}} = \ker \tau_{\mathrm{N}} = \operatorname{dom} A_{\mathrm{N}}.$$

As a consequence of Theorem 8.3.9 and Theorem 8.3.10 one can also extend the second Green identity in (8.2.19) to elements $f \in \operatorname{dom} T_{\max}$ and $g \in H^2(\Omega)$.

Corollary 8.3.11. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain, and let*

$$\widetilde{\tau}_{\mathrm{D}} : \operatorname{dom} T_{\max} \to H^{-1/2}(\partial\Omega) \quad \textit{and} \quad \widetilde{\tau}_{\mathrm{N}} : \operatorname{dom} T_{\max} \to H^{-3/2}(\partial\Omega)$$

be the unique continuous extensions of the Dirichlet and Neumann trace operators

$$\tau_{\mathrm{D}} : H^2(\Omega) \to H^{3/2}(\partial\Omega) \quad \textit{and} \quad \tau_{\mathrm{N}} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$$

from Theorem 8.3.9 and Theorem 8.3.10, respectively. Then the second Green identity in (8.2.19) extends to

$$\begin{aligned}&(T_{\max} f, g)_{L^2(\Omega)} - (f, T_{\max} g)_{L^2(\Omega)} \\ &\qquad = \langle \widetilde{\tau}_{\mathrm{D}} f, \tau_{\mathrm{N}} g\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} - \langle \widetilde{\tau}_{\mathrm{N}} f, \tau_{\mathrm{D}} g\rangle_{H^{-3/2}(\partial\Omega)\times H^{3/2}(\partial\Omega)}\end{aligned}$$

for $f \in \operatorname{dom} T_{\max}$ and $g \in H^2(\Omega)$.

Proof. Let $f \in \operatorname{dom} T_{\max}$ and $g \in H^2(\Omega)$. Since $C^\infty(\overline{\Omega})$ is dense in $\operatorname{dom} T_{\max}$ with respect to the graph norm by Lemma 8.3.8 and $C^\infty(\overline{\Omega}) \subset H^2(\Omega) \subset \operatorname{dom} T_{\max}$, there exists a sequence $(f_n) \subset H^2(\Omega)$ such that $f_n \to f$ and $T_{\max} f_n \to T_{\max} f$

in $L^2(\Omega)$. Moreover, $\tau_D f_n \to \widetilde{\tau}_D f$ in $H^{-1/2}(\partial\Omega)$ and $\tau_N f_n \to \widetilde{\tau}_N f$ in $H^{-3/2}(\partial\Omega)$, because $\widetilde{\tau}_D$ and $\widetilde{\tau}_N$ are continuous with respect to the graph norm. Therefore, with the help of the second Green identity (8.2.19), one concludes that

$$\begin{aligned}
&(T_{\max} f, g)_{L^2(\Omega)} - (f, T_{\max} g)_{L^2(\Omega)} \\
&\quad = \lim_{n\to\infty} (T_{\max} f_n, g)_{L^2(\Omega)} - \lim_{n\to\infty} (f_n, T_{\max} g)_{L^2(\Omega)} \\
&\quad = \lim_{n\to\infty} \big[(\tau_D f_n, \tau_N g)_{L^2(\partial\Omega)} - (\tau_N f_n, \tau_D g)_{L^2(\partial\Omega)}\big] \\
&\quad = \lim_{n\to\infty} \big[\langle \tau_D f_n, \tau_N g\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} - \langle \tau_N f_n, \tau_D g\rangle_{H^{-3/2}(\partial\Omega)\times H^{3/2}(\partial\Omega)}\big] \\
&\quad = \langle \widetilde{\tau}_D f, \tau_N g\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} - \langle \widetilde{\tau}_N f, \tau_D g\rangle_{H^{-3/2}(\partial\Omega)\times H^{3/2}(\partial\Omega)},
\end{aligned}$$

which completes the proof. □

Note that, by construction, there exists a bounded right inverse for the extended Dirichlet trace operator $\widetilde{\tau}_D$ (see (8.3.16)–(8.3.17)) and similarly there exists a bounded right inverse for the extended Neumann trace operator $\widetilde{\tau}_N$. This also implies that the Dirichlet-to-Neumann map in Definition 8.3.6 admits a natural extension to a bounded mapping from from $H^{-1/2}(\partial\Omega)$ into $H^{-3/2}(\partial\Omega)$.

Corollary 8.3.12. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain and let $\widetilde{\tau}_D$ and $\widetilde{\tau}_N$ be the unique continuous extensions of the Dirichlet and Neumann trace operators from Theorem 8.3.9 and Theorem 8.3.10, respectively. Then for $\lambda \in \rho(A_D)$ the Dirichlet-to-Neumann map in Definition 8.3.6 admits an extension to a bounded operator*

$$\widetilde{D}(\lambda) : H^{-1/2}(\partial\Omega) \to H^{-3/2}(\partial\Omega), \qquad \widetilde{\tau}_D f_\lambda \mapsto \widetilde{\tau}_N f_\lambda,$$

where $f_\lambda \in \mathfrak{N}_\lambda(T_{\max})$.

For later purposes the following fact is provided.

Proposition 8.3.13. *The minimal operator $T_{\min}$ in (8.3.2) is simple.*

Proof. Since A_D is a self-adjoint extension of $T_{\min}$ with discrete spectrum, it suffices to check that $T_{\min}$ has no eigenvalues; cf. Proposition 3.4.8. For this, assume that $T_{\min} f = \lambda f$ for some $\lambda \in \mathbb{R}$ and some $f \in \operatorname{dom} T_{\min}$. Since $\operatorname{dom} T_{\min} = H^2_0(\Omega)$, there exist $(f_k) \in C_0^\infty(\Omega)$ such that $f_k \to f$ in $H^2(\Omega)$. Denote the zero extensions of f and f_k to all of $\mathbb{R}^n$ by $\widetilde{f}$ and $\widetilde{f}_k$, respectively. Then $\widetilde{f}_k \to \widetilde{f}$ in $L^2(\mathbb{R}^n)$ and for all $h \in C_0^\infty(\mathbb{R}^n)$ and $\alpha \in \mathbb{N}_0^n$ such that $|\alpha| \leq 2$ one computes

$$\begin{aligned}
\int_{\mathbb{R}^n} \widetilde{f}(x) D^\alpha h(x)\,dx &= \lim_{k\to\infty} \int_{\mathbb{R}^n} \widetilde{f}_k(x) D^\alpha h(x)\,dx \\
&= (-1)^{|\alpha|} \lim_{k\to\infty} \int_{\mathbb{R}^n} (D^\alpha \widetilde{f}_k)(x) h(x)\,dx \\
&= (-1)^{|\alpha|} \lim_{k\to\infty} \int_{\Omega} (D^\alpha f_k)(x) h(x)\,dx
\end{aligned}$$

$$= (-1)^{|\alpha|} \int_\Omega (D^\alpha f)(x) h(x)\,dx$$
$$= (-1)^{|\alpha|} \int_{\mathbb{R}^n} \widetilde{(D^\alpha f)}(x) h(x)\,dx,$$

where $\widetilde{(D^\alpha f)}$ denotes the zero extension of $D^\alpha f$ to all of $\mathbb{R}^n$. It follows from this computation that

$$D^\alpha \widetilde{f} = \widetilde{(D^\alpha f)} \in L^2(\mathbb{R}^n), \qquad |\alpha| \leq 2,$$

and hence $\widetilde{f} \in H^2(\mathbb{R}^n)$. Furthermore, if $\widetilde{V} \in L^\infty(\mathbb{R}^n)$ denotes some real extension of V, then $(-\Delta + \widetilde{V})\widetilde{f} = \lambda \widetilde{f}$ and since $\widetilde{f}$ vanishes on an open subset of $\mathbb{R}^n$, the unique continuation principle (see, e.g., [652, Theorem XIII.63]) implies $\widetilde{f} = 0$, so that $f = 0$. Therefore, $T_{\min}$ has no eigenvalues and now Proposition 3.4.8 shows that $T_{\min}$ is simple. □

8.4 A boundary triplet for the maximal Schrödinger operator

In this section a boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ for the maximal operator $T_{\max}$ in (8.3.3) is provided under the assumption that $\Omega \subset \mathbb{R}^n$ is a bounded C^2-domain. The corresponding Weyl function is closely connected to the extended Dirichlet-to-Neumann map in Corollary 8.3.12. As examples, Neumann and Robin type boundary conditions are discussed, and it is also explained that there exist self-adjoint realizations of $-\Delta + V$ in $L^2(\Omega)$ which are not semibounded and which may have essential spectrum of rather arbitrary form.

Recall from Corollary 8.2.2 that

$$\{H^{1/2}(\partial\Omega),\, L^2(\partial\Omega), H^{-1/2}(\partial\Omega)\}$$

is a Gelfand triple and there exist isometric isomorphisms $\iota_\pm : H^{\pm\frac{1}{2}}(\partial\Omega) \to L^2(\partial\Omega)$ such that

$$\langle \varphi, \psi \rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} = (\iota_- \varphi, \iota_+ \psi)_{L^2(\partial\Omega)}$$

holds for all $\varphi \in H^{-1/2}(\partial\Omega)$ and $\psi \in H^{1/2}(\partial\Omega)$. For the definition of the boundary mappings in the next proposition recall also the definition and the properties of the Dirichlet operator A_{D} (see Theorem 8.3.4), as well as the direct sum decomposition

$$\operatorname{dom} T_{\max} = \operatorname{dom} A_{\mathrm{D}} \dotplus \mathfrak{N}_\eta(T_{\max}), \tag{8.4.1}$$

which holds for all $\eta \in \rho(A_{\mathrm{D}})$. In particular, since A_{D} is semibounded from below, one may choose $\eta \in \rho(A_{\mathrm{D}}) \cap \mathbb{R}$ in (8.4.1). Further, let $\tau_{\mathrm{N}} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$ be the Neumann trace operator in (8.2.12) and let $\widetilde{\tau}_{\mathrm{D}} : \operatorname{dom} T_{\max} \to H^{-1/2}(\partial\Omega)$ be the extension of the Dirichlet trace operator in Theorem 8.3.9.

Theorem 8.4.1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let A_D be the self-adjoint Dirichlet realization of $-\Delta + V$ in $L^2(\Omega)$ in Theorem 8.3.4, fix $\eta \in \rho(A_D) \cap \mathbb{R}$, and decompose $f \in \operatorname{dom} T_{\max}$ according to (8.4.1) in the form $f = f_D + f_\eta$, where $f_D \in \operatorname{dom} A_D$ and $f_\eta \in \mathfrak{N}_\eta(T_{\max})$. Then $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$, where*

$$\Gamma_0 f = \iota_- \widetilde{\tau}_D f \quad \textit{and} \quad \Gamma_1 f = -\iota_+ \tau_N f_D, \qquad f = f_D + f_\eta \in \operatorname{dom} T_{\max},$$

is a boundary triplet for $(T_{\min})^* = T_{\max}$ such that

$$A_0 = A_D \qquad \textit{and} \qquad A_1 = T_{\min} \,\widehat{+}\, \widehat{\mathfrak{N}}_\eta(T_{\max}). \tag{8.4.2}$$

Proof. Let $f, g \in \operatorname{dom} T_{\max}$ and decompose f and g in the form $f = f_D + f_\eta$ and $g = g_D + g_\eta$ with $f_D, g_D \in \operatorname{dom} A_D \subset H^2(\Omega)$ and $f_\eta, g_\eta \in \mathfrak{N}_\eta(T_{\max})$. Since A_D is self-adjoint,

$$(T_{\max} f_D, g_D)_{L^2(\Omega)} = (A_D f_D, g_D)_{L^2(\Omega)} = (f_D, A_D\, g_D)_{L^2(\Omega)} = (f_D, T_{\max}\, g_D)_{L^2(\Omega)}$$

and since η is real, one also has

$$(T_{\max} f_\eta, g_\eta)_{L^2(\Omega)} = (\eta f_\eta, g_\eta)_{L^2(\Omega)} = (f_\eta, \eta g_\eta)_{L^2(\Omega)} = (f_\eta, T_{\max}\, g_\eta)_{L^2(\Omega)}.$$

Therefore, one obtains

$$\begin{aligned}
&(T_{\max} f, g)_{L^2(\Omega)} - (f, T_{\max}\, g)_{L^2(\Omega)} \\
&\quad = \big(T_{\max}(f_D + f_\eta), g_D + g_\eta\big)_{L^2(\Omega)} - \big(f_D + f_\eta, T_{\max}(g_D + g_\eta)\big)_{L^2(\Omega)} \\
&\quad = (T_{\max} f_\eta, g_D)_{L^2(\Omega)} + (T_{\max} f_D, g_\eta)_{L^2(\Omega)} \\
&\qquad\quad - (f_\eta, T_{\max}\, g_D)_{L^2(\Omega)} - (f_D, T_{\max}\, g_\eta)_{L^2(\Omega)}.
\end{aligned}$$

Let $\widetilde{\tau}_N$ be the extension of the Neumann trace to $\operatorname{dom} T_{\max}$ from Theorem 8.3.10. Then it follows together with Corollary 8.3.11 and $\tau_D f_D = \tau_D g_D = 0$ that

$$\begin{aligned}
&(T_{\max} f_\eta, g_D)_{L^2(\Omega)} - (f_\eta, T_{\max}\, g_D)_{L^2(\Omega)} \\
&\quad = \langle \widetilde{\tau}_D f_\eta, \tau_N g_D \rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} - \langle \widetilde{\tau}_N f_\eta, \tau_D g_D \rangle_{H^{-3/2}(\partial\Omega)\times H^{3/2}(\partial\Omega)} \\
&\quad = \langle \widetilde{\tau}_D f_\eta, \tau_N g_D \rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)}
\end{aligned}$$

and

$$\begin{aligned}
&(T_{\max} f_D, g_\eta)_{L^2(\Omega)} - (f_D, T_{\max} g_\eta)_{L^2(\Omega)} \\
&\quad = \langle \tau_D f_D, \widetilde{\tau}_N g_\eta \rangle_{H^{3/2}(\partial\Omega)\times H^{-3/2}(\partial\Omega)} - \langle \tau_N f_D, \widetilde{\tau}_D g_\eta \rangle_{H^{1/2}(\partial\Omega)\times H^{-1/2}(\partial\Omega)} \\
&\quad = -\langle \tau_N f_D, \widetilde{\tau}_D g_\eta \rangle_{H^{1/2}(\partial\Omega)\times H^{-1/2}(\partial\Omega)}.
\end{aligned}$$

Hence,

$$\begin{aligned}
&(T_{\max} f, g)_{L^2(\Omega)} - (f, T_{\max} g)_{L^2(\Omega)} \\
&\quad = \langle \widetilde{\tau}_D f_\eta, \tau_N g_D \rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)} - \langle \tau_N f_D, \widetilde{\tau}_D g_\eta \rangle_{H^{1/2}(\partial\Omega)\times H^{-1/2}(\partial\Omega)} \\
&\quad = \big(\iota_- \widetilde{\tau}_D f_\eta, \iota_+ \tau_N g_D\big)_{L^2(\partial\Omega)} - \big(\iota_+ \tau_N f_D, \iota_- \widetilde{\tau}_D g_\eta\big)_{L^2(\partial\Omega)}
\end{aligned}$$

and, since $f_{\rm D}, g_{\rm D} \in \ker \tau_{\rm D} = \ker \widetilde{\tau}_{\rm D}$ according to Theorem 8.3.9, one sees that

$$\begin{aligned}(T_{\max} f, g)_{L^2(\Omega)} &- (f, T_{\max} g)_{L^2(\Omega)} \\ &= \bigl(\iota_- \widetilde{\tau}_{\rm D} f, \iota_+ \tau_{\rm N} g_{\rm D}\bigr)_{L^2(\partial\Omega)} - \bigl(\iota_+ \tau_{\rm N} f_{\rm D}, \iota_- \widetilde{\tau}_{\rm D} g\bigr)_{L^2(\partial\Omega)} \\ &= \bigl(-\iota_+ \tau_{\rm N} f_{\rm D}, \iota_- \widetilde{\tau}_{\rm D} g\bigr)_{L^2(\partial\Omega)} - \bigl(\iota_- \widetilde{\tau}_{\rm D} f, -\iota_+ \tau_{\rm N} g_{\rm D}\bigr)_{L^2(\partial\Omega)} \\ &= (\Gamma_1 f, \Gamma_0 g)_{L^2(\partial\Omega)} - (\Gamma_0 f, \Gamma_1 g)_{L^2(\partial\Omega)}\end{aligned}$$

for all $f, g \in \operatorname{dom} T_{\max}$, that is, the abstract Green identity is satisfied. To verify the surjectivity of the mapping

$$\begin{pmatrix}\Gamma_0 \\ \Gamma_1\end{pmatrix} : \operatorname{dom} T_{\max} \to L^2(\partial\Omega) \times L^2(\partial\Omega), \tag{8.4.3}$$

let $\varphi, \psi \in L^2(\partial\Omega)$ and consider $\iota_-^{-1}\varphi \in H^{-1/2}(\partial\Omega)$ and $-\iota_+^{-1}\psi \in H^{1/2}(\partial\Omega)$. Observe that by (8.2.12) the Neumann trace operator $\tau_{\rm N}$ is a surjective mapping from $\{h \in H^2(\Omega) : \tau_{\rm D} h = 0\}$ onto $H^{1/2}(\partial\Omega)$, that is, $\tau_{\rm N} : \operatorname{dom} A_{\rm D} \to H^{1/2}(\partial\Omega)$ is onto, and hence there exists $f_{\rm D} \in \operatorname{dom} A_{\rm D}$ such that $\tau_{\rm N} f_{\rm D} = -\iota_+^{-1}\psi$. Next recall from Theorem 8.3.9 that the extended Dirichlet trace operator $\widetilde{\tau}_{\rm D}$ maps $\operatorname{dom} T_{\max}$ onto $H^{-1/2}(\partial\Omega)$ and that $\ker \widetilde{\tau}_{\rm D} = \ker \tau_{\rm D} = \operatorname{dom} A_{\rm D}$. Hence, it follows from the direct sum decomposition $\operatorname{dom} T_{\max} = \operatorname{dom} A_{\rm D} + \mathfrak{N}_\eta(T_{\max})$ that the restriction $\widetilde{\tau}_{\rm D} : \mathfrak{N}_\eta(T_{\max}) \to H^{-1/2}(\partial\Omega)$ is bijective, in particular, there exists $f_\eta \in \mathfrak{N}_\eta(T_{\max})$ such that $\widetilde{\tau}_{\rm D} f_\eta = \iota_-^{-1}\varphi$. Now it follows that $f := f_{\rm D} + f_\eta \in \operatorname{dom} T_{\max}$ satisfies

$$\Gamma_0 f = \iota_- \widetilde{\tau}_{\rm D} f = \iota_- \widetilde{\tau}_{\rm D} f_\eta = \iota_- \iota_-^{-1}\varphi = \varphi$$

and

$$\Gamma_1 f = -\iota_+ \tau_{\rm N} f_{\rm D} = \iota_+ \iota_+^{-1}\psi = \psi,$$

and hence the mapping in (8.4.3) is onto. Thus, $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ is a boundary triplet for $(T_{\min})^* = T_{\max}$, as claimed.

From the definition of Γ_0 and $\ker \widetilde{\tau}_{\rm D} = \ker \tau_{\rm D} = \operatorname{dom} A_{\rm D}$ it is clear that $\operatorname{dom} A_{\rm D} = \ker \Gamma_0$, and hence the self-adjoint extension corresponding to Γ_0 coincides with the Dirichlet operator $A_{\rm D}$, that is, the first identity in (8.4.2) holds. It remains to check the second identity in (8.4.2). For this let $f = f_{\rm D} + f_\eta \in \ker \Gamma_1$, which means $\tau_{\rm N} f_{\rm D} = 0$. Thus, $f_{\rm D} \in \operatorname{dom} T_{\min}$ by (8.2.15) and it follows that $A_1 \subset T_{\min} \,\widehat{+}\, \widehat{\mathfrak{N}}_\eta(T_{\max})$. The inclusion $T_{\min} \,\widehat{+}\, \widehat{\mathfrak{N}}_\eta(T_{\max}) \subset A_1$ is clear from the definition of Γ_1. This leads to the second identity in (8.4.2). □

Remark 8.4.2. The boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in Theorem 8.4.1 is closely related to the boundary triplet $\{\mathfrak{N}_\eta(T_{\max}), \Gamma_0', \Gamma_1'\}$ in Corollary 5.5.12, where

$$\Gamma_0' f = f_\eta \quad \text{and} \quad \Gamma_1' f = P_{\mathfrak{N}_\eta(T_{\max})}(A_{\rm D} - \eta) f_{\rm D}, \quad f = f_{\rm D} + f_\eta \in \operatorname{dom} T_{\max}.$$

In fact, one has $\ker \Gamma_0 = \ker \Gamma_0'$ and $\ker \Gamma_1 = \ker \Gamma_1'$, and hence

$$\begin{pmatrix}\Gamma_0' \\ \Gamma_1'\end{pmatrix} = \begin{pmatrix} W_{11} & 0 \\ 0 & W_{22}\end{pmatrix}\begin{pmatrix}\Gamma_0 \\ \Gamma_1\end{pmatrix}$$

with some 2×2 operator matrix $\mathcal{W} = (W_{ij})_{i,j=1}^2$ as in Theorem 2.5.1, see also Corollary 2.5.5. In the present situation it follows from Theorem 8.3.9 and (8.4.1) that the restriction $\iota_- \widetilde{\tau}_D : \mathfrak{N}_\eta(T_{\max}) \to L^2(\partial\Omega)$ is bijective and one concludes $W_{11} = (\iota_- \widetilde{\tau}_D)^{-1}$. Now the properties of $\mathcal{W}$ imply that $W_{22} = (\iota_- \widetilde{\tau}_D)^*$.

With the help of the extended Dirichlet-to-Neumann map in Corollary 8.3.12 one obtains a more explicit description of the domain of the self-adjoint operator A_1 in (8.4.2).

Proposition 8.4.3. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let A_D be the self-adjoint Dirichlet realization of $-\Delta + V$ in $L^2(\Omega)$, and fix $\eta \in \rho(A_D) \cap \mathbb{R}$. Moreover, let $\widetilde{D}(\eta)$ be the extended Dirichlet-to-Neumann map in Corollary 8.3.12. Then the self-adjoint extension A_1 of $T_{\min}$ in (8.4.2) is defined on*

$$\operatorname{dom} A_1 = \bigl\{ f \in \operatorname{dom} T_{\max} : \widetilde{\tau}_N f = \widetilde{D}(\eta) \widetilde{\tau}_D f \bigr\}. \tag{8.4.4}$$

In the case that $\eta < m(A_D)$, where $m(A_D)$ denotes the lower bound of A_D, the operator A_1 coincides with the Kreĭn type extension $S_{K,\eta}$ of $T_{\min}$ in Definition 5.4.2. In particular, if $m(A_D) > 0$ and $\eta = 0$, then $A_1 = S_{K,0}$ is the Kreĭn–von Neumann extension of $T_{\min}$.

Proof. It is clear from Theorem 8.4.1 that

$$\operatorname{dom} A_1 = \ker \Gamma_1 = \bigl\{ f = f_D + f_\eta \in \operatorname{dom} T_{\max} : \tau_N f_D = 0 \bigr\}.$$

Let $\widetilde{\tau}_N$ be the extension of the Neumann trace τ_N to the maximal domain in Theorem 8.3.10. Then the boundary condition $\tau_N f_D = 0$ can be rewritten as $\widetilde{\tau}_N f = \widetilde{\tau}_N f_\eta$, where $f = f_D + f_\eta \in \operatorname{dom} T_{\max}$. With the help of the extended Dirichlet-to-Neumann map

$$\widetilde{D}(\eta) : H^{-1/2}(\partial\Omega) \to H^{-3/2}(\partial\Omega), \quad \widetilde{\tau}_D f_\eta \mapsto \widetilde{\tau}_N f_\eta, \qquad f_\eta \in \mathfrak{N}_\eta(T_{\max}),$$

one obtains $\widetilde{\tau}_N f_\eta = \widetilde{D}(\eta) \widetilde{\tau}_D f_\eta = \widetilde{D}(\eta) \widetilde{\tau}_D f$, which implies (8.4.4).

If $\eta \in \mathbb{R}$ is chosen smaller than the lower bound $m(A_D)$ of A_D, then it follows from the second identity in (8.4.2), Lemma 5.4.1, and Definition 5.4.2 that the Kreĭn type extension $S_{K,\eta} = T_{\min} \,\widehat{+}\, \widehat{\mathfrak{N}}_\eta(T_{\max})$ of $T_{\min}$ and A_1 coincide. In the special case $m(A_D) > 0$ and $\eta = 0$ one has $A_1 = S_{K,0}$, which is the Kreĭn–von Neumann extension of $T_{\min}$; cf. Definition 5.4.2. □

In the next proposition the γ-field and the Weyl function corresponding to the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in Theorem 8.4.1 are provided. Note that for $f = f_D + f_\eta$ decomposed as in (8.4.1) one has

$$\Gamma_0 f = \iota_- \widetilde{\tau}_D f = \iota_- \widetilde{\tau}_D f_\eta,$$

as $\ker \widetilde{\tau}_D = \ker \tau_D = \operatorname{dom} A_D$ by Theorem 8.3.9. It is also clear from (8.4.1) that Γ_0 is a bijective mapping from $\mathfrak{N}_\eta(T_{\max})$ onto $L^2(\partial\Omega)$.

Proposition 8.4.4. *Let $\{L^2(\partial\Omega),\Gamma_0,\Gamma_1\}$ be the boundary triplet for $(T_{\min})^* = T_{\max}$ in Theorem 8.4.1 and let $f_\eta(\varphi)$ be the unique element in $\mathfrak{N}_\eta(T_{\max})$ such that $\Gamma_0 f_\eta(\varphi) = \varphi$. Then for all $\lambda \in \rho(A_{\rm D})$ the γ-field corresponding to the boundary triplet $\{L^2(\partial\Omega),\Gamma_0,\Gamma_1\}$ is given by*

$$\gamma(\lambda)\varphi = \bigl(I + (\lambda-\eta)(A_{\rm D}-\lambda)^{-1}\bigr) f_\eta(\varphi), \quad \varphi \in L^2(\partial\Omega), \tag{8.4.5}$$

and $f_\lambda(\varphi) := \gamma(\lambda)\varphi$ is the unique element in $\mathfrak{N}_\lambda(T_{\max})$ such that $\Gamma_0 f_\lambda(\varphi) = \varphi$. Furthermore, one has

$$\gamma(\lambda)^* = -\iota_+\tau_{\rm N}(A_{\rm D}-\bar\lambda)^{-1}, \quad \lambda \in \rho(A_{\rm D}). \tag{8.4.6}$$

The Weyl function M corresponding to the boundary triplet $\{L^2(\partial\Omega),\Gamma_0,\Gamma_1\}$ is given by

$$M(\lambda)\varphi = (\eta-\lambda)\iota_+\tau_{\rm N}(A_{\rm D}-\lambda)^{-1} f_\eta(\varphi), \quad \varphi \in L^2(\partial\Omega).$$

In particular, $\gamma(\eta)\varphi = f_\eta(\varphi)$ and $M(\eta)\varphi = 0$ for all $\varphi \in L^2(\partial\Omega)$.

Proof. Since by definition $\gamma(\eta)$ is the inverse of the restriction of Γ_0 to $\mathfrak{N}_\eta(T_{\max})$, it is clear that $\gamma(\eta)\varphi = f_\eta(\varphi)$, where $f_\eta(\varphi)$ is the unique element in $\mathfrak{N}_\eta(T_{\max})$ such that $\Gamma_0 f_\eta(\varphi) = \varphi$. Both (8.4.5) and (8.4.6) are consequences of Proposition 2.3.2. In order to compute the Weyl function note that

$$\gamma(\lambda)\varphi = f_\eta(\varphi) + (\lambda-\eta)(A_{\rm D}-\lambda)^{-1} f_\eta(\varphi)$$

is decomposed in $(\lambda-\eta)(A_{\rm D}-\lambda)^{-1} f_\eta(\varphi) \in \operatorname{dom} A_{\rm D}$ and $f_\eta(\varphi) \in \mathfrak{N}_\eta(T_{\max})$, and hence by the definition of Γ_1 it follows that

$$\begin{aligned} M(\lambda)\varphi = \Gamma_1\gamma(\lambda)\varphi &= -\iota_+\tau_{\rm N}\bigl[(\lambda-\eta)(A_{\rm D}-\lambda)^{-1} f_\eta(\varphi)\bigr] \\ &= (\eta-\lambda)\iota_+\tau_{\rm N}(A_{\rm D}-\lambda)^{-1} f_\eta(\varphi). \end{aligned}$$

The assertion $M(\eta)\varphi = 0$ for all $\varphi \in L^2(\partial\Omega)$ is clear from the above. □

The Weyl function M in Proposition 8.4.4 is closely connected with the Dirichlet-to-Neumann map $D(\lambda)$ and its extension $\widetilde D(\lambda)$, $\lambda \in \rho(A_{\rm D})$, in Definition 8.3.6 and Corollary 8.3.12. This connection will be made explicit in the next lemma. First, consider $f = f_{\rm D} + f_\eta \in \operatorname{dom} T_{\max}$ as in (8.4.1). In the present situation one has

$$\tau_{\rm N} f_{\rm D} = \widetilde\tau_{\rm N} f_{\rm D} = \widetilde\tau_{\rm N} f - \widetilde\tau_{\rm N} f_\eta.$$

Hence, making use of $\widetilde D(\eta)\widetilde\tau_{\rm D} f_\eta = \widetilde\tau_{\rm N} f_\eta$ (see Corollary 8.3.12) and the identity $\ker \widetilde\tau_{\rm D} = \operatorname{dom} A_{\rm D}$, it follows that

$$\tau_{\rm N} f_{\rm D} = \widetilde\tau_{\rm N} f - \widetilde D(\eta)\widetilde\tau_{\rm D} f_\eta = \widetilde\tau_{\rm N} f - \widetilde D(\eta)\widetilde\tau_{\rm D} f. \tag{8.4.7}$$

Lemma 8.4.5. *Let M be the Weyl function corresponding to the boundary triplet in Theorem 8.4.1 and let $\widetilde{D}(\lambda)$, $\lambda \in \rho(A_{\mathrm{D}})$, be the extended Dirichlet-to-Neumann map in Corollary 8.3.12. Then the regularization property*

$$\operatorname{ran}\big(\widetilde{D}(\eta) - \widetilde{D}(\lambda)\big) \subset H^{1/2}(\partial\Omega) \tag{8.4.8}$$

holds and one has

$$M(\lambda)\varphi = \iota_+\big(\widetilde{D}(\eta) - \widetilde{D}(\lambda)\big)\iota_-^{-1}\varphi, \qquad \varphi \in L^2(\partial\Omega), \tag{8.4.9}$$

and

$$M(\lambda)\varphi = \iota_+\big(D(\eta) - D(\lambda)\big)\iota_-^{-1}\varphi, \qquad \varphi \in H^2(\partial\Omega), \tag{8.4.10}$$

Proof. For $\psi \in H^{-1/2}(\partial\Omega)$ choose $f_\lambda \in \mathfrak{N}_\lambda(T_{\max})$ such that $\widetilde{\tau}_{\mathrm{D}} f_\lambda = \psi$ or, equivalently, $\Gamma_0 f_\lambda = \iota_-\psi$. Decompose f_λ in the form $f_\lambda = f_{\mathrm{D}}^\lambda + f_{\lambda,\eta}$ with $f_{\mathrm{D}}^\lambda \in \operatorname{dom} A_{\mathrm{D}}$ and $f_{\lambda,\eta} \in \mathfrak{N}_\eta(T_{\max})$. Then one computes

$$\big(\widetilde{D}(\eta) - \widetilde{D}(\lambda)\big)\psi = \widetilde{D}(\eta)\widetilde{\tau}_{\mathrm{D}} f_\lambda - \widetilde{\tau}_{\mathrm{N}} f_\lambda = -\tau_{\mathrm{N}} f_{\mathrm{D}}^\lambda, \tag{8.4.11}$$

where (8.4.7) was used in the last step for $f = f_\lambda$. Since $f_{\mathrm{D}}^\lambda \in \operatorname{dom} A_{\mathrm{D}} \subset H^2(\Omega)$, the regularization property (8.4.8) follows from (8.2.12). From (8.4.11) one also concludes that

$$\iota_+\big(\widetilde{D}(\eta) - \widetilde{D}(\lambda)\big)\iota_-^{-1}\Gamma_0 f_\lambda = -\iota_+\tau_{\mathrm{N}} f_{\mathrm{D}}^\lambda = \Gamma_1 f_\lambda,$$

and since $M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda$ by the definition of the Weyl function, this shows (8.4.9).

It remains to prove the second assertion (8.4.10). For this note that the restriction of $\iota_-^{-1} : L^2(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ to $H^2(\partial\Omega)$ is an isometric isomorphism from $H^2(\partial\Omega)$ onto $H^{3/2}(\partial\Omega)$ by Corollary 8.2.2. Furthermore, it follows from the definition that the extended Dirichlet-to-Neumann map $\widetilde{D}(\lambda)$ coincides with the Dirichlet-to-Neumann map $D(\lambda)$ on $H^{3/2}(\partial\Omega)$. With these observations it is clear that (8.4.10) follows when restricting (8.4.9) to $H^2(\partial\Omega)$. □

Remark 8.4.6. The boundary mappings in Theorem 8.4.1 and the corresponding γ-field and Weyl function depend on the choice of $\eta \in \rho(A_{\mathrm{D}}) \cap \mathbb{R}$ and the decomposition of $f \in \operatorname{dom} T_{\max}$ as $f = f_{\mathrm{D}}^\eta + f_\eta$; observe that also $f_{\mathrm{D}} = f_{\mathrm{D}}^\eta \in \operatorname{dom} A_{\mathrm{D}}$ depends on η. Suppose now that the boundary mappings are defined with respect to some other $\eta' \in \rho(A_{\mathrm{D}}) \cap \mathbb{R}$ and decompose f accordingly as $f = f_{\mathrm{D}}^{\eta'} + f_{\eta'}$. If $\Gamma_0^\eta, \Gamma_1^\eta$ denote the boundary mappings in Theorem 8.4.1 with respect to η, and $\Gamma_0^{\eta'}, \Gamma_1^{\eta'}$ denote the boundary mappings in Theorem 8.4.1 with respect to η', then one has

$$\begin{pmatrix} \Gamma_0^{\eta'} \\ \Gamma_1^{\eta'} \end{pmatrix} = \begin{pmatrix} I & 0 \\ -M(\eta') & I \end{pmatrix} \begin{pmatrix} \Gamma_0^{\eta} \\ \Gamma_1^{\eta} \end{pmatrix}. \tag{8.4.12}$$

In fact, that $\Gamma_0^{\eta'} f = \Gamma_0^{\eta} f$ for $f \in \operatorname{dom} T_{\max}$ is clear from Theorem 8.4.1, and for the remaining identity in (8.4.12) it follows from Lemma 8.4.5 that

$$\begin{aligned}
-M(\eta')\Gamma_0^{\eta} f + \Gamma_1^{\eta} f &= \iota_+ \bigl(\widetilde{D}(\eta') - \widetilde{D}(\eta)\bigr)\iota_-^{-1}\Gamma_0^{\eta} f + \Gamma_1^{\eta} f \\
&= \iota_+ \bigl(\widetilde{D}(\eta')\widetilde{\tau}_{\mathrm{D}} f - \widetilde{D}(\eta)\widetilde{\tau}_{\mathrm{D}} f\bigr) - \iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}}^{\eta} \\
&= \iota_+ \bigl(\widetilde{D}(\eta')\widetilde{\tau}_{\mathrm{D}} f_{\eta'} - \widetilde{D}(\eta)\widetilde{\tau}_{\mathrm{D}} f_{\eta}\bigr) - \iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}}^{\eta} \\
&= \iota_+ \bigl(\widetilde{\tau}_{\mathrm{N}} f_{\eta'} - \widetilde{\tau}_{\mathrm{N}} f_{\eta}\bigr) - \iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}}^{\eta} \\
&= \iota_+ \tau_{\mathrm{N}} \bigl(f_{\mathrm{D}}^{\eta} - f_{\mathrm{D}}^{\eta'}\bigr) - \iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}}^{\eta} \\
&= \Gamma_1^{\eta'} f.
\end{aligned}$$

Finally, note that the γ-fields and Weyl functions of the boundary triplets in Theorem 8.4.1 for different η and η' transform accordingly; cf. Proposition 2.5.3.

Next some classes of extensions of $T_{\min}$ and their spectral properties are briefly discussed. Let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet in Theorem 8.4.1 with corresponding γ-field γ and Weyl function M in Proposition 8.4.4. According to Corollary 2.1.4, the self-adjoint (maximal dissipative, maximal accumulative) extensions $A_\Theta \subset T_{\max}$ of $T_{\min}$ are in a one-to-one correspondence to the self-adjoint (maximal dissipative, maximal accumulative) relations Θ in $L^2(\partial\Omega)$ via

$$\begin{aligned}
\operatorname{dom} A_\Theta &= \bigl\{ f \in \operatorname{dom} T_{\max} : \{\Gamma_0 f, \Gamma_1 f\} \in \Theta \bigr\} \\
&= \bigl\{ f \in \operatorname{dom} T_{\max} : \{\iota_- \widetilde{\tau}_{\mathrm{D}} f, -\iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}}\} \in \Theta \bigr\}.
\end{aligned} \tag{8.4.13}$$

If Θ is an operator in $L^2(\partial\Omega)$, then the domain of A_Θ is given by

$$\operatorname{dom} A_\Theta = \bigl\{ f \in \operatorname{dom} T_{\max} : \Theta \iota_- \widetilde{\tau}_{\mathrm{D}} f = -\iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}} \bigr\}. \tag{8.4.14}$$

Let Θ be a self-adjoint relation in $L^2(\partial\Omega)$ and let A_Θ be the corresponding self-adjoint realization of $-\Delta + V$ in $L^2(\Omega)$. By Corollary 1.10.9, Θ can be represented in terms of bounded operators $\mathcal{A}, \mathcal{B} \in \mathbf{B}(L^2(\partial\Omega))$ satisfying the conditions $\mathcal{A}^*\mathcal{B} = \mathcal{B}^*\mathcal{A}$, $\mathcal{A}\mathcal{B}^* = \mathcal{B}\mathcal{A}^*$, and $\mathcal{A}^*\mathcal{A} + \mathcal{B}^*\mathcal{B} = I = \mathcal{A}\mathcal{A}^* + \mathcal{B}\mathcal{B}^*$ such that

$$\Theta = \bigl\{ \{\mathcal{A}\varphi, \mathcal{B}\varphi\} : \varphi \in L^2(\partial\Omega) \bigr\} = \bigl\{ \{\psi, \psi'\} : \mathcal{A}^*\psi' = \mathcal{B}^*\psi \bigr\}.$$

In this case one has

$$\operatorname{dom} A_\Theta = \bigl\{ f \in \operatorname{dom} T_{\max} : -\mathcal{A}^* \iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}} = \mathcal{B}^* \iota_- \widetilde{\tau}_{\mathrm{D}} f \bigr\},$$

and for $\lambda \in \rho(A_\Theta) \cap \rho(A_{\mathrm{D}})$ the Kreĭn formula for the corresponding resolvents

$$\begin{aligned}
(A_\Theta - \lambda)^{-1} &= (A_{\mathrm{D}} - \lambda)^{-1} + \gamma(\lambda)\bigl(\Theta - M(\lambda)\bigr)^{-1}\gamma(\bar{\lambda})^* \\
&= (A_{\mathrm{D}} - \lambda)^{-1} + \gamma(\lambda)\mathcal{A}\bigl(\mathcal{B} - M(\lambda)\mathcal{A}\bigr)^{-1}\gamma(\bar{\lambda})^*
\end{aligned} \tag{8.4.15}$$

holds by Theorem 2.6.1 and Corollary 2.6.3. Recall that in the present situation the spectrum of $A_{\rm D} = A_0$ is discrete by Proposition 8.3.2. According to Theorem 2.6.2, $\lambda \in \rho(A_{\rm D})$ is an eigenvalue of A_Θ if and only if $\ker(\Theta - M(\lambda))$ or, equivalently, $\ker(\mathcal{B} - M(\lambda)\mathcal{A})$ is nontrivial, and that

$$\ker(A_\Theta - \lambda) = \gamma(\lambda)\ker\bigl(\Theta - M(\lambda)\bigr) = \gamma(\lambda)\mathcal{A}\ker\bigl(\mathcal{B} - M(\lambda)\mathcal{A}\bigr).$$

Although Ω is a bounded C^2-domain, it will turn out in Example 8.4.9 that the spectrum of A_Θ is in general not discrete, and thus continuous spectrum may be present. It then follows from Theorem 2.6.2 and Theorem 2.6.5 that $\lambda \in \rho(A_{\rm D})$ belongs to the continuous spectrum $\sigma_{\rm c}(A_\Theta)$ (essential spectrum $\sigma_{\rm ess}(A_\Theta)$ or discrete spectrum $\sigma_{\rm d}(A_\Theta)$) of A_Θ if and only if 0 belongs to $\sigma_{\rm c}(\Theta - M(\lambda))$ ($\sigma_{\rm ess}(\Theta - M(\lambda))$ or $\sigma_{\rm d}(\Theta - M(\lambda))$).

For a complete description of the spectrum of A_Θ recall that the symmetric operator $T_{\min}$ is simple according to Proposition 8.3.13 and make use of a transform of the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ as in Chapter 3.8. This reasoning implies that λ is an eigenvalue of A_Θ if and only if λ is a pole of the function

$$\lambda \mapsto M_\Theta(\lambda) = \bigl(\mathcal{A}^* + \mathcal{B}^* M(\lambda)\bigr)\bigl(\mathcal{B}^* - \mathcal{A}^* M(\lambda)\bigr)^{-1}.$$

It is important to note in this context that the multiplicity of the eigenvalues of A_Θ is not necessarily finite and that the dimension of the eigenspace $\ker(A_\Theta - \lambda)$ of an isolated eigenvalue λ of A_Θ coincides with the dimension of the range of the residue of M_Θ at λ. Furthermore, the continuous and absolutely continuous spectrum of A_Θ can be characterized as in Section 3.8, e.g., one has

$$\sigma_{\rm ac}(A_\Theta) = \overline{\bigcup_{\varphi \in L^2(\partial\Omega)} \operatorname{clos}_{\rm ac}\Bigl(\bigl\{x \in \mathbb{R} : 0 < \operatorname{Im}\bigl(M_\Theta(x + i0)\varphi, \varphi\bigr)_{L^2(\partial\Omega)} < \infty\bigr\}\Bigr)}.$$

In the special case that the self-adjoint relation Θ in $L^2(\partial\Omega)$ is a bounded operator the boundary condition reads as in (8.4.14) and according to Section 3.8 the spectral properties of the self-adjoint operator A_Θ can also be described with the help of the function

$$\lambda \mapsto \bigl(\Theta - M(\lambda)\bigr)^{-1}.$$

The general boundary conditions in (8.4.13) and (8.4.14) contain also typical classes of boundary conditions that are treated in spectral problems for partial differential operators, as, e.g., Neumann or Robin type boundary conditions. In the following example the standard Neumann boundary conditions are discussed. Note that the Neumann operator does not coincide with the Kreĭn type extension $S_{{\rm K},\eta}$ or the Kreĭn–von Neumann extension $S_{{\rm K},0}$ of $T_{\min}$ in Proposition 8.4.3.

Example 8.4.7. Let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet in Theorem 8.4.1 and choose $\eta \in \rho(A_{\rm D}) \cap \mathbb{R}$ in (8.4.1) in such a way that also $\eta \in \rho(A_{\rm N})$, where

A_{N} denotes the Neumann realization of $-\Delta + V$ in Proposition 8.3.3 and Theorem 8.3.4. Since both self-adjoint operators A_{D} and A_{N} are semibounded from below (or both have discrete spectrum), such an η exists. In this situation it follows that the Dirichlet-to-Neumann map

$$D(\eta) : H^{3/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$$

in Definition 8.3.6 is a bijective mapping. Furthermore, $\iota_+ : H^{1/2}(\partial\Omega) \to L^2(\partial\Omega)$ is bijective and the restriction of $\iota_-^{-1} : L^2(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ to $H^2(\partial\Omega)$ is an isometric isomorphism from $H^2(\partial\Omega)$ onto $H^{3/2}(\partial\Omega)$ according to Corollary 8.2.2. Hence, it is clear that

$$\Theta_{\mathrm{N}} := \iota_+ D(\eta)\iota_-^{-1}, \qquad \operatorname{dom}\Theta_{\mathrm{N}} := H^2(\partial\Omega), \tag{8.4.16}$$

is a densely defined bijective operator in $L^2(\partial\Omega)$. Furthermore, for $\varphi \in H^2(\partial\Omega)$ and $\psi = \iota_-^{-1}\varphi \in H^{3/2}(\partial\Omega)$ it follows from Corollary 8.2.2 that

$$\big(\iota_+ D(\eta)\iota_-^{-1}\varphi, \varphi\big)_{L^2(\partial\Omega)} = \big(\iota_+ D(\eta)\psi, \iota_-\psi\big)_{L^2(\partial\Omega)} = (D(\eta)\psi, \psi)_{L^2(\partial\Omega)}. \tag{8.4.17}$$

Now choose $f_\eta \in H^2(\Omega)$ such that $(-\Delta + V)f_\eta = \eta f_\eta$ and $\tau_{\mathrm{D}} f_\eta = \psi$, which is possible by (8.3.9) and (8.2.12). Then it follows from Definition 8.3.6 and the first Green identity in (8.2.18) that

$$\begin{aligned} (D(\eta)\psi, \psi)_{L^2(\partial\Omega)} &= \big(D(\eta)\tau_{\mathrm{D}} f_\eta, \tau_{\mathrm{D}} f_\eta\big)_{L^2(\partial\Omega)} \\ &= (\tau_{\mathrm{N}} f_\eta, \tau_{\mathrm{D}} f_\eta)_{L^2(\partial\Omega)} \\ &= \|\nabla f_\eta\|^2_{L^2(\Omega;\mathbb{C}^n)} + (\Delta f_\eta, f_\eta)_{L^2(\Omega)} \\ &= \|\nabla f_\eta\|^2_{L^2(\Omega;\mathbb{C}^n)} + ((V-\eta) f_\eta, f_\eta)_{L^2(\Omega)}, \end{aligned} \tag{8.4.18}$$

so that $(D(\eta)\psi, \psi)_{L^2(\partial\Omega)} \in \mathbb{R}$ and hence $(\Theta_{\mathrm{N}}\varphi, \varphi)_{L^2(\partial\Omega)} \in \mathbb{R}$ by (8.4.16)–(8.4.17) for all $\varphi \in H^2(\partial\Omega)$. It follows that the bijective operator Θ_{N} is symmetric in $L^2(\partial\Omega)$, and hence Θ_{N} is an unbounded self-adjoint operator in $L^2(\partial\Omega)$ such that $0 \in \rho(\Theta_{\mathrm{N}})$.

The self-adjoint realization of $-\Delta + V$ in $L^2(\Omega)$ corresponding to the self-adjoint operator Θ_{N} in (8.4.16) is denoted by $A_{\Theta_{\mathrm{N}}}$. A function $f \in \operatorname{dom} T_{\max}$ belongs to $\operatorname{dom} A_{\Theta_{\mathrm{N}}}$ if and only if

$$\Gamma_0 f = \iota_- \widetilde{\tau}_{\mathrm{D}} f \in \operatorname{dom}\Theta_{\mathrm{N}} \quad \text{and} \quad \Gamma_1 f = \Theta_{\mathrm{N}}\Gamma_0 f.$$

Note that $\iota_- \widetilde{\tau}_{\mathrm{D}} f \in \operatorname{dom}\Theta_{\mathrm{N}}$ forces $\widetilde{\tau}_{\mathrm{D}} f \in H^{3/2}(\partial\Omega)$ and hence $f \in H^2(\Omega)$ and $\widetilde{\tau}_{\mathrm{D}} f = \tau_{\mathrm{D}} f$ by (8.2.12) and Theorem 8.3.9. It then follows from (8.4.7) and (8.4.16) that the boundary condition $\Gamma_1 f = \Theta_{\mathrm{N}}\Gamma_0 f$ takes on the form

$$\iota_+ D(\eta)\tau_{\mathrm{D}} f - \iota_+ \tau_{\mathrm{N}} f = -\iota_+ \tau_{\mathrm{N}} f_{\mathrm{D}} = \Gamma_1 f = \Theta_{\mathrm{N}}\Gamma_0 f = \iota_+ D(\eta)\tau_{\mathrm{D}} f,$$

that is, $\tau_{\rm N} f = 0$. Hence, it has been shown that $\operatorname{dom} A_{\Theta_{\rm N}} \subset H^2(\Omega)$ and that $\tau_{\rm N} f = 0$ for all $f \in \operatorname{dom} A_{\Theta_{\rm N}}$. Therefore, $A_{\Theta_{\rm N}} \subset A_{\rm N}$ and since both operators are self-adjoint one concludes that $A_{\Theta_{\rm N}} = A_{\rm N}$.

Note also that by (8.4.16) and Lemma 8.4.5 one has

$$\big(\Theta_{\rm N} - M(\lambda)\big)\varphi = \iota_+ D(\eta)\iota_-^{-1}\varphi - \iota_+\big(D(\eta) - D(\lambda)\big)\iota_-^{-1}\varphi = \iota_+ D(\lambda)\iota_-^{-1}\varphi$$

for $\varphi \in H^2(\partial\Omega)$ and $\lambda \in \rho(A_{\rm D})$. Hence, it follows that $\Theta_{\rm N} - M(\lambda)$ is a bijective operator in $L^2(\partial\Omega)$ for all $\lambda \in \rho(A_{\rm D}) \cap \rho(A_{\rm N})$ which is defined on $H^2(\partial\Omega)$. Therefore, (8.4.15) implies that the resolvents of $A_{\rm D}$ and $A_{\rm N}$ are related via

$$(A_{\rm N} - \lambda)^{-1} = (A_{\rm D} - \lambda)^{-1} + \gamma(\lambda)\iota_- D(\lambda)^{-1}\iota_+^{-1}\gamma(\bar\lambda)^*,$$

where γ is the γ-field corresponding to the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in Proposition 8.4.4.

The next example is a generalization of the previous example from Neumann to local and nonlocal Robin boundary conditions.

Example 8.4.8. Let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be as in the previous example and fix some $\eta \in \rho(A_{\rm D}) \cap \rho(A_{\rm N}) \cap \mathbb{R}$. Then the operator $\Theta_{\rm N} = \iota_+ D(\eta)\iota_-^{-1}$ in (8.4.16) is an unbounded self-adjoint operator in $L^2(\partial\Omega)$ with domain $H^2(\partial\Omega)$, and $0 \in \rho(\Theta_{\rm N})$. Assume that

$$B : H^{3/2}(\partial\Omega) \to H^{1/2}(\partial\Omega) \tag{8.4.19}$$

is compact as an operator from $H^{3/2}(\partial\Omega)$ into $H^{1/2}(\partial\Omega)$ and that B is symmetric in $L^2(\partial\Omega)$, that is, $(B\psi, \psi)_{L^2(\partial\Omega)} \in \mathbb{R}$ for all $\psi \in \operatorname{dom} B = H^{3/2}(\partial\Omega)$. Then it follows that

$$\iota_+ B\iota_-^{-1} : H^2(\partial\Omega) \to L^2(\partial\Omega)$$

is compact as an operator from $H^2(\partial\Omega)$ into $L^2(\partial\Omega)$ and as in (8.4.17) one sees that $\iota_+ B\iota_-^{-1}$ is symmetric in $L^2(\partial\Omega)$. Consider the operator

$$\Theta_B := \iota_+\big(D(\eta) - B\big)\iota_-^{-1} = \Theta_{\rm N} - \iota_+ B\iota_-^{-1}, \quad \operatorname{dom}\Theta_B = H^2(\partial\Omega), \tag{8.4.20}$$

and observe that the symmetric operator $\iota_+ B\iota_-^{-1}$ is a relative compact perturbation of the self-adjoint operator $\Theta_{\rm N}$ in $L^2(\partial\Omega)$, that is, the operator

$$\iota_+ B\iota_-^{-1}\Theta_{\rm N}^{-1}$$

is compact in $L^2(\partial\Omega)$. It is well known from standard perturbation results (see, e.g., [652, Corollary 2 of Theorem XIII.14]) that in this case the perturbed operator Θ_B is self-adjoint in $L^2(\partial\Omega)$.

The self-adjoint realization of $-\Delta + V$ in $L^2(\Omega)$ corresponding to the self-adjoint operator Θ_B in (8.4.20) is denoted by A_{Θ_B}. It is clear that a function $f \in \operatorname{dom} T_{\max}$ belongs to $\operatorname{dom} A_{\Theta_B}$ if and only if

$$\Gamma_0 f = \iota_-\widetilde\tau_{\rm D} f \in \operatorname{dom}\Theta_B \quad \text{and} \quad \Gamma_1 f = \Theta_B\Gamma_0 f. \tag{8.4.21}$$

In the same way as in Example 8.4.7 the fact that $\iota_-\widetilde{\tau}_{\rm D} f \in \operatorname{dom}\Theta_B$ implies that $f \in H^2(\Omega)$ and $\widetilde{\tau}_{\rm D} f = \tau_{\rm D} f$, and the boundary condition $\Gamma_1 f = \Theta_B \Gamma_0 f$ takes the explicit form

$$\iota_+ D(\eta)\tau_{\rm D} f - \iota_+\tau_{\rm N} f = \Gamma_1 f = \Theta_B\Gamma_0 f = \iota_+\big(D(\eta) - B\big)\tau_{\rm D} f,$$

that is, $\tau_{\rm N} f = B\tau_{\rm D} f$. Conversely, if $f \in H^2(\Omega)$ is such that $\tau_{\rm N} f = B\tau_{\rm D} f$, then f satisfies (8.4.21) and hence $f \in \operatorname{dom} A_{\Theta_B}$. Thus, it has been shown that the self-adjoint operator A_{Θ_B} is defined on

$$\operatorname{dom} A_{\Theta_B} = \big\{ f \in H^2(\Omega) : \tau_{\rm N} f = B\tau_{\rm D} f \big\}.$$

In the same way as in the previous example one obtains

$$\Theta_B - M(\lambda) = \iota_+\big(D(\lambda) - B\big)\iota_-^{-1}$$

and hence for all $\lambda \in \rho(A_{\rm D}) \cap \rho(A_{\Theta_B})$ one has

$$(A_{\Theta_B} - \lambda)^{-1} = (A_{\rm D} - \lambda)^{-1} + \gamma(\lambda)\iota_-\big(D(\lambda) - B\big)^{-1}\iota_+^{-1}\gamma(\bar\lambda)^*.$$

Finally, note that a sufficient condition for the operator B in (8.4.19) to be compact is that $B : H^{3/2}(\partial\Omega) \to H^{1/2+\varepsilon}(\partial\Omega)$ is bounded for some $\varepsilon > 0$, or that $B : H^{3/2-\varepsilon'}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ is bounded for some $\varepsilon' > 0$, since the embeddings $H^{1/2+\varepsilon}(\partial\Omega) \hookrightarrow H^{1/2}(\partial\Omega)$ and $H^{3/2}(\partial\Omega) \hookrightarrow H^{3/2-\varepsilon'}(\partial\Omega)$ are compact by (8.2.8).

In the next example it is shown that the (essential) spectrum of a self-adjoint realization A_Θ of $-\Delta + V$ can be very general, depending on the properties of the parameter Θ. In particular, the self-adjoint realization A_Θ may not be semibounded.

Example 8.4.9. Let $\eta \in \rho(A_{\rm D}) \cap \mathbb{R}$, consider an arbitrary self-adjoint operator Ξ in the Hilbert space $\mathfrak{N}_\eta(T_{\max}) = \ker(T_{\max} - \eta)$, and assume that $\eta \in \rho(\Xi)$. Denote by $P_{\mathfrak{N}_\eta}$ the orthogonal projection in $L^2(\Omega)$ onto $\mathfrak{N}_\eta(T_{\max})$ and let $\iota_{\mathfrak{N}_\eta}$ be the natural embedding of $\mathfrak{N}_\eta(T_{\max})$ into $L^2(\Omega)$.

Let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet in Theorem 8.4.1 with corresponding γ-field and Weyl function in Proposition 8.4.4. Note that $M(\eta) = 0$ and that both

$$P_{\mathfrak{N}_\eta}\gamma(\eta) : L^2(\partial\Omega) \to \mathfrak{N}_\eta(T_{\max}) \quad \text{and} \quad \gamma(\eta)^*\iota_{\mathfrak{N}_\eta} : \mathfrak{N}_\eta(T_{\max}) \to L^2(\partial\Omega)$$

are isomorphisms. It follows that

$$\Theta := \big(\gamma(\eta)^*\iota_{\mathfrak{N}_\eta}\big)(\Xi - \eta)\big(P_{\mathfrak{N}_\eta}\gamma(\eta)\big)$$

is a self-adjoint operator in $L^2(\partial\Omega)$ with $0 \in \rho(\Theta)$ and

$$\Theta^{-1} = \big(P_{\mathfrak{N}_\eta}\gamma(\eta)\big)^{-1}(\Xi - \eta)^{-1}\big(\gamma(\eta)^*\iota_{\mathfrak{N}_\eta}\big)^{-1}. \tag{8.4.22}$$

Let A_Θ be the corresponding self-adjoint realization of $-\Delta+V$ in (8.4.13)–(8.4.14) defined on

$$\operatorname{dom} A_\Theta = \bigl\{ f \in \operatorname{dom} T_{\max} : \Theta\iota_- \widetilde{\tau}_{\rm D} f = -\iota_+ \tau_{\rm N} f_{\rm D} \bigr\}.$$

Since $M(\eta) = 0$ and $\eta \in \mathbb{R}$, Kreĭn's formula in (8.4.15) takes the form

$$\begin{aligned}(A_\Theta - \eta)^{-1} &= (A_{\rm D} - \eta)^{-1} + \gamma(\eta)\Theta^{-1}\gamma(\eta)^* \\ &= (A_{\rm D} - \lambda)^{-1} + \begin{pmatrix} P_{\mathfrak{N}_\eta}\gamma(\eta)\Theta^{-1}\gamma(\eta)^*\iota_{\mathfrak{N}_\eta} & 0 \\ 0 & 0 \end{pmatrix},\end{aligned}$$

where the block operator matrix is acting with respect to the space decomposition $L^2(\Omega) = \mathfrak{N}_\eta(T_{\max}) \oplus (\mathfrak{N}_\eta(T_{\max}))^\perp$. Using (8.4.22) one then concludes that

$$(A_\Theta - \eta)^{-1} = (A_{\rm D} - \eta)^{-1} + \begin{pmatrix} (\Xi - \eta)^{-1} & 0 \\ 0 & 0 \end{pmatrix}.$$

In particular, since $(A_{\rm D} - \eta)^{-1}$ is compact, well-known perturbation results show that

$$\sigma_{\rm ess}\bigl((A_\Theta - \eta)^{-1}\bigr) = \sigma_{\rm ess}\bigl((\Xi - \eta)^{-1}\bigr) \cup \{0\},$$

and hence $\sigma_{\rm ess}(A_\Theta) = \sigma_{\rm ess}(\Xi)$.

8.5 Semibounded Schrödinger operators

The semibounded self-adjoint realizations of $-\Delta + V$, where $V \in L^\infty(\Omega)$ is real, and the corresponding densely defined closed semibounded forms in $L^2(\Omega)$ are described in this section. For this purpose it is convenient to construct a boundary pair which is compatible with the boundary triplet in Theorem 8.4.1 and to apply the general results from Section 5.6. Under the additional assumption that $V \geq 0$, the nonnegative realizations of $-\Delta + V$ and the corresponding nonnegative forms in $L^2(\Omega)$ are discussed as a special case. In this situation the Kreĭn–von Neumann extension appears as the smallest nonnegative extension.

Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain and let $A_{\rm D}$ be the self-adjoint Dirichlet realization of $-\Delta + V$. It is clear from Proposition 8.3.2 that $A_{\rm D}$ coincides with the Friedrichs extension of the minimal operator $T_{\min}$ in (8.3.2) and that $A_{\rm D}$ is bounded from below with lower bound $m(A_{\rm D}) > v_-$, where $v_- = \operatorname{essinf} V$. Furthermore, the resolvent of $A_{\rm D}$ is compact since the domain Ω is bounded. Therefore, the following description of the semibounded self-adjoint extensions of $T_{\min}$ is an immediate consequence of Proposition 5.5.6 and Proposition 5.5.8.

Proposition 8.5.1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet for $(T_{\min})^* = T_{\max}$ from Theorem 8.4.1, and let*

$$\begin{aligned} A_\Theta &= -\Delta + V, \\ \operatorname{dom} A_\Theta &= \bigl\{ f \in \operatorname{dom} T_{\max} : \{\Gamma_0 f, \Gamma_1 f\} \in \Theta \bigr\}, \end{aligned}$$

be a self-adjoint extension of $T_{\min}$ in $L^2(\Omega)$ corresponding to a self-adjoint relation Θ in $L^2(\partial\Omega)$ as in (8.4.13). Then

$$A_\Theta \text{ is semibounded} \quad \Leftrightarrow \quad \Theta \text{ is semibounded.}$$

Recall also from Section 8.3 that the densely defined closed semibounded form $\mathfrak{t}_{A_\mathrm{D}}$ corresponding to A_D is defined on $H_0^1(\Omega)$. Now fix some $\eta < m(A_\mathrm{D})$, use the direct sum decomposition

$$\operatorname{dom} T_{\max} = \mathfrak{N}_\eta(T_{\max}) \dotplus \operatorname{dom} A_\mathrm{D} = \mathfrak{N}_\eta(T_{\max}) \dotplus \big(H^2(\Omega) \cap H_0^1(\Omega)\big) \tag{8.5.1}$$

from (8.4.1) and Proposition 8.3.2, and consider the corresponding boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ for $(T_{\min})^* = T_{\max}$ in Theorem 8.4.1 given by

$$\Gamma_0 f = \iota_- \widetilde{\tau}_\mathrm{D} f \quad \text{and} \quad \Gamma_1 f = -\iota_+ \tau_\mathrm{N} f_\mathrm{D}, \tag{8.5.2}$$

where $f = f_\eta + f_\mathrm{D} \in \operatorname{dom} T_{\max}$ with $f_\eta \in \mathfrak{N}_\eta(T_{\max})$ and $f_\mathrm{D} \in \operatorname{dom} A_\mathrm{D}$; cf. (8.5.1). It is clear that $A_0 = A_\mathrm{D}$ coincides with the Friedrichs extension of $T_{\min}$ and $A_1 = T_{\min} \widehat{+} \widehat{\mathfrak{N}}_\eta(T_{\max})$ coincides with the Kreĭn type extension $S_{\mathrm{K},\eta}$ of $T_{\min}$; cf. Definition 5.4.2. In order to define a boundary pair for $T_{\min}$ corresponding to $A_1 = S_{\mathrm{K},\eta}$, consider the densely defined closed semibounded form $\mathfrak{t}_{S_{\mathrm{K},\eta}}$ associated with $S_{\mathrm{K},\eta}$ and recall from Corollary 5.4.16 the direct sum decomposition

$$\operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}} = \mathfrak{N}_\eta(T_{\max}) \dotplus \operatorname{dom} \mathfrak{t}_{A_\mathrm{D}} = \mathfrak{N}_\eta(T_{\max}) \dotplus H_0^1(\Omega) \tag{8.5.3}$$

of $\operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}}$. Comparing (8.5.1) and (8.5.3) one sees that $\operatorname{dom} T_{\max} \subset \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}}$ and that the domain of the Dirichlet operator A_D in (8.5.1) is replaced by the corresponding form domain in (8.5.3). The functions $f \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}}$ will be written in the form $f = f_\eta + f_\mathrm{F}$, where $f_\eta \in \mathfrak{N}_\eta(T_{\max})$ and $f_\mathrm{F} \in \operatorname{dom} \mathfrak{t}_{A_\mathrm{D}} = H_0^1(\Omega)$. Now define the mapping

$$\Lambda : \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}} \to L^2(\partial\Omega), \quad f \mapsto \Lambda f = \iota_- \widetilde{\tau}_\mathrm{D} f_\eta. \tag{8.5.4}$$

It will be shown next that $\{L^2(\partial\Omega), \Lambda\}$ is a boundary pair that is compatible with the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in the sense of Definition 5.6.4; although the main part of the proof of Lemma 8.5.2 is similar to Example 5.6.9, the details are provided.

Lemma 8.5.2. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain and let A_D be the self-adjoint Dirichlet realization of $-\Delta + V$ with lower bound $m(A_\mathrm{D})$. Fix $\eta < m(A_\mathrm{D})$, let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the corresponding boundary triplet for $(T_{\min})^* = T_{\max}$ from Theorem 8.4.1, and let Λ be the mapping in (8.5.4). Then $\{L^2(\partial\Omega), \Lambda\}$ is a boundary pair for $T_{\min}$ corresponding to the Kreĭn type extension $S_{\mathrm{K},\eta}$ which is compatible with the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$. Moreover, one has*

$$(T_{\max} f, g)_{L^2(\Omega)} = \mathfrak{t}_{S_{\mathrm{K},\eta}}[f, g] + (\Gamma_1 f, \Lambda g)_{L^2(\partial\Omega)} \tag{8.5.5}$$

for all $f \in \operatorname{dom} T_{\max}$ and $g \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}}$.

Proof. According to Lemma 5.6.5 (ii), it suffices to show that for some $a < \eta$ the mapping Λ in (8.5.4) is bounded from the Hilbert space

$$\mathfrak{H}_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} = \big(\operatorname{dom}\mathfrak{t}_{S_{\mathrm{K},\eta}}, (\cdot,\cdot)_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a}\big)$$

to $L^2(\partial\Omega)$ and that Λ extends the mapping Γ_0 in (8.5.2). In the present situation it is clear that the compatibility condition $A_1 = S_{\mathrm{K},\eta}$ is satisfied.

In order to show that Λ is bounded fix some $a < \eta$, recall first from (5.1.7) that the Hilbert space norm on $\mathfrak{H}_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a}$ is given by

$$\|f\|^2_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} = \mathfrak{t}_{S_{\mathrm{K},\eta}}[f] - a\|f\|^2_{L^2(\Omega)}, \quad f \in \operatorname{dom}\mathfrak{t}_{S_{\mathrm{K},\eta}} = \mathfrak{H}_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a}.$$

It follows from Theorem 8.3.9 that the restriction $\iota_-\widetilde{\tau}_{\mathrm{D}} : \mathfrak{N}_\eta(T_{\max}) \to L^2(\partial\Omega)$ is bounded and hence for $f = f_\eta + f_{\mathrm{F}} \in \operatorname{dom}\mathfrak{t}_{S_{\mathrm{K},\eta}}$, decomposed according to (8.5.3) in $f_\eta \in \mathfrak{N}_\eta(T_{\max})$ and $f_{\mathrm{F}} \in \operatorname{dom}\mathfrak{t}_{A_{\mathrm{D}}}$, one has the estimate

$$\|\Lambda f\|^2_{L^2(\partial\Omega)} = \|\iota_-\widetilde{\tau}_{\mathrm{D}} f_\eta\|^2_{L^2(\partial\Omega)} \le C\|f_\eta\|^2_{L^2(\Omega)}. \tag{8.5.6}$$

Now the orthogonal sum decomposition

$$\operatorname{dom}\mathfrak{t}_{S_{\mathrm{K},\eta}} = \mathfrak{N}_a(T_{\max}) \oplus_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} \operatorname{dom}\mathfrak{t}_{A_{\mathrm{D}}} \tag{8.5.7}$$

from Corollary 5.4.15 will be used. To this end, define

$$f_a := \big(I + (a-\eta)(A_{\mathrm{D}} - a)^{-1}\big) f_\eta$$

and note that $f = f_a + h_{\mathrm{F}}$ with $f_a \in \mathfrak{N}_a(T_{\max})$ and $h_{\mathrm{F}} = f_\eta - f_a + f_{\mathrm{F}} \in \operatorname{dom}\mathfrak{t}_{A_{\mathrm{D}}}$. Then one has

$$f_\eta = \big(I + (\eta - a)(A_{\mathrm{D}} - \eta)^{-1}\big) f_a$$

and Proposition 1.4.6 leads to the estimate

$$\|f_\eta\|_{L^2(\Omega)} \le \frac{m(A_{\mathrm{D}}) - a}{m(A_{\mathrm{D}}) - \eta}\,\|f_a\|_{L^2(\Omega)}. \tag{8.5.8}$$

Furthermore, it follows from (5.1.9) and the orthogonal sum decomposition (8.5.7) that

$$(\eta - a)\|f_a\|^2_{L^2(\Omega)} \le \|f_a\|^2_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} \le \|f_a\|^2_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} + \|h_{\mathrm{F}}\|^2_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} = \|f\|^2_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a}.$$

From this estimate, (8.5.6), and (8.5.8) one concludes that $\Lambda : \mathfrak{H}_{\mathfrak{t}_{S_{\mathrm{K},\eta}}-a} \to L^2(\partial\Omega)$ is bounded.

From the definition of Λ in (8.5.4) and the decompositions (8.5.1) and (8.5.3) it is clear that Λ is an extension of the mapping Γ_0 in (8.5.2). Moreover, by construction, the condition $A_1 = S_{\mathrm{K},\eta}$ is satisfied. Therefore, Lemma 5.6.5 (ii) shows that $\{L^2(\partial\Omega), \Lambda\}$ is a boundary pair for $T_{\min}$ corresponding to $S_{\mathrm{K},\eta}$ which is compatible with the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$. The identity (8.5.5) follows from Corollary 5.6.7. □

The next theorem is a variant of Theorem 5.6.13 in the present situation.

Theorem 8.5.3. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let A_{D} be the self-adjoint Dirichlet realization of $-\Delta + V$ with lower bound $m(A_{\mathrm{D}})$, and fix $\eta < m(A_{\mathrm{D}})$. Let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet for $(T_{\min})^* = T_{\max}$ from Theorem 8.4.1 and let $\{L^2(\partial\Omega), \Lambda\}$ be the compatible boundary pair in Lemma 8.5.2. Furthermore, let Θ be a semibounded self-adjoint relation in $L^2(\partial\Omega)$ and let A_Θ be the corresponding semibounded self-adjoint extension of $T_{\min}$ in Proposition 8.5.1. Then the closed semibounded form ω_Θ in $L^2(\partial\Omega)$ corresponding to Θ and the densely defined closed semibounded form $\mathfrak{t}_{A_\Theta}$ corresponding to A_Θ are related by*

$$\begin{aligned} \mathfrak{t}_{A_\Theta}[f,g] &= \mathfrak{t}_{S_{\mathrm{K},\eta}}[f,g] + \omega_\Theta[\Lambda f, \Lambda g], \\ \operatorname{dom} \mathfrak{t}_{A_\Theta} &= \bigl\{ f \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}} : \Lambda f \in \operatorname{dom} \omega_\Theta \bigr\}. \end{aligned} \tag{8.5.9}$$

For completeness, the form $\mathfrak{t}_{A_\Theta}$ in Theorem 8.5.3 will be made more explicit using Corollary 5.6.14. First note that, by the definition of the boundary map Λ in (8.5.4) and the decomposition (8.5.3), one can rewrite (8.5.9) as

$$\begin{aligned} \mathfrak{t}_{A_\Theta}[f,g] &= \mathfrak{t}_{S_{\mathrm{K},\eta}}[f,g] + \omega_\Theta[\iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta, \iota_- \widetilde{\tau}_{\mathrm{D}} g_\eta], \\ \operatorname{dom} \mathfrak{t}_{A_\Theta} &= \bigl\{ f = f_\eta + f_{\mathrm{F}} \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}} : \iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta \in \operatorname{dom} \omega_\Theta \bigr\}. \end{aligned} \tag{8.5.10}$$

If $m(\Theta)$ denotes the lower bound of the semibounded self-adjoint relation Θ and $\mu \leq m(\Theta)$ is fixed, then the closed semibounded form $\mathfrak{t}_{A_\Theta}$ in (8.5.9)–(8.5.10) corresponding to A_Θ is given by

$$\begin{aligned} \mathfrak{t}_{A_\Theta}[f,g] &= \mathfrak{t}_{S_{\mathrm{K},\eta}}[f,g] + \bigl((\Theta_{\mathrm{op}} - \mu)^{\frac12} \iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta, (\Theta_{\mathrm{op}} - \mu)^{\frac12} \iota_- \widetilde{\tau}_{\mathrm{D}} g_\eta \bigr)_{L^2(\partial\Omega)} \\ &\qquad + \mu \, (\iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta, \iota_- \widetilde{\tau}_{\mathrm{D}} g_\eta)_{L^2(\partial\Omega)}, \\ \operatorname{dom} \mathfrak{t}_{A_\Theta} &= \bigl\{ f = f_\eta + f_{\mathrm{F}} \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}} : \iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta \in \operatorname{dom} (\Theta_{\mathrm{op}} - \mu)^{\frac12} \bigr\}; \end{aligned}$$

as usual, here Θ_{op} denotes the semibounded self-adjoint operator part of Θ acting in $L^2(\partial\Omega)_{\mathrm{op}} = \overline{\operatorname{dom}}\, \Theta$. In the special case where $\Theta_{\mathrm{op}} \in \mathbf{B}(L^2(\partial\Omega)_{\mathrm{op}})$ one has

$$\begin{aligned} \mathfrak{t}_{A_\Theta}[f,g] &= \mathfrak{t}_{S_{\mathrm{K},\eta}}[f,g] + \bigl(\Theta_{\mathrm{op}} \, \iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta, \iota_- \widetilde{\tau}_{\mathrm{D}} g_\eta \bigr)_{L^2(\partial\Omega)}, \\ \operatorname{dom} \mathfrak{t}_{A_\Theta} &= \bigl\{ f = f_\eta + f_{\mathrm{F}} \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}} : \iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta \in \operatorname{dom} \Theta_{\mathrm{op}} \bigr\}, \end{aligned}$$

and if $\Theta \in \mathbf{B}(L^2(\partial\Omega))$, then

$$\mathfrak{t}_{A_\Theta}[f,g] = \mathfrak{t}_{S_{\mathrm{K},\eta}}[f,g] + \bigl(\Theta \iota_- \widetilde{\tau}_{\mathrm{D}} f_\eta, \iota_- \widetilde{\tau}_{\mathrm{D}} g_\eta \bigr)_{L^2(\partial\Omega)}, \qquad \operatorname{dom} \mathfrak{t}_{A_\Theta} = \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},\eta}}.$$

Recall also from Corollary 5.4.15 that the form $\mathfrak{t}_{S_{\mathrm{K},\eta}}$ can be expressed in terms of the form $\mathfrak{t}_{A_{\mathrm{D}}}$ and the resolvent of A_{D}.

Finally, the special case $V \geq 0$ will be briefly considered. In this situation the minimal operator $T_{\min}$ and the Dirichlet operator A_{D} are both uniformly positive and hence in the above construction of a boundary triplet and corresponding boundary pair one may choose $\eta = 0$. More precisely, Theorem 8.4.1 has the following form.

Corollary 8.5.4. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let $A_{\rm D}$ be the self-adjoint Dirichlet realization of $-\Delta+V$ in $L^2(\Omega)$ with $V \geq 0$, and decompose $f \in \operatorname{dom} T_{\max}$ according to (8.4.1) with $\eta = 0$ in the form $f = f_{\rm D} + f_0$, where $f_{\rm D} \in \operatorname{dom} A_{\rm D}$ and $f_0 \in \ker T_{\max}$. Then $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$, where*

$$\Gamma_0 f = \iota_- \widetilde{\tau}_{\rm D} f \quad \textit{and} \quad \Gamma_1 f = -\iota_+ \tau_{\rm N} f_{\rm D}, \qquad f = f_{\rm D} + f_0 \in \operatorname{dom} T_{\max},$$

is a boundary triplet for $(T_{\min})^* = T_{\max}$ such that

$$A_0 = A_{\rm D} \qquad \textit{and} \qquad A_1 = T_{\min} \,\widehat{+}\, \widehat{\mathfrak{N}}_0(T_{\max})$$

coincide with the Friedrichs extension and the Kreĭn–von Neumann extension of $T_{\min}$, respectively.

It is clear from Proposition 8.4.4 that for all $\lambda \in \rho(A_{\rm D})$ the γ-field and Weyl function corresponding to the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in Corollary 8.5.4 have the form

$$\gamma(\lambda)\varphi = \bigl(I + \lambda(A_{\rm D} - \lambda)^{-1}\bigr) f_0(\varphi), \quad \varphi \in L^2(\partial\Omega),$$

and

$$M(\lambda)\varphi = -\iota_+ \tau_{\rm N} \lambda (A_{\rm D} - \lambda)^{-1} f_0(\varphi), \quad \varphi \in L^2(\partial\Omega), \tag{8.5.11}$$

respectively, where $f_0(\varphi)$ is the unique element in $\mathfrak{N}_0(T_{\max})$ with the property that $\Gamma_0 f_0(\varphi) = \iota_- \widetilde{\tau}_{\rm D} f_0(\varphi) = \varphi$.

The next proposition is a variant of Proposition 8.5.1 for nonnegative extensions.

Proposition 8.5.5. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, assume that $V \geq 0$, and let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet for $(T_{\min})^* = T_{\max}$ from Corollary 8.5.4. Let*

$$A_\Theta = -\Delta + V,$$
$$\operatorname{dom} A_\Theta = \bigl\{ f \in \operatorname{dom} T_{\max} : \{\Gamma_0 f, \Gamma_1 f\} \in \Theta \bigr\},$$

be a self-adjoint extension of $T_{\min}$ in $L^2(\Omega)$ corresponding to a self-adjoint relation Θ in $L^2(\partial\Omega)$ as in (8.4.13). Then

$$A_\Theta \ \textit{is nonnegative} \quad \Leftrightarrow \quad \Theta \ \textit{is nonnegative.}$$

Proof. Note that the Weyl function M in (8.5.11) satisfies $M(0) = 0$ and that $T_{\min}$ is uniformly positive. Therefore, if A_Θ is a nonnegative self-adjoint extension of $T_{\min}$, then Proposition 5.5.6 with $x = 0$ shows that the self-adjoint relation Θ in $L^2(\partial\Omega)$ is nonnegative. Conversely, if Θ is a nonnegative self-adjoint relation in $L^2(\partial\Omega)$, then it follows from Corollary 5.5.15 and $A_1 = S_{{\rm K},0} \geq 0$ that A_Θ is a nonnegative self-adjoint extension of $T_{\min}$. □

In the nonnegative case the boundary mapping Λ in (8.5.4) is given by

$$\Lambda : \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},0}} \to L^2(\partial\Omega), \quad f \mapsto \Lambda f = \iota_- \widetilde{\tau}_{\mathrm{D}} f_0, \tag{8.5.12}$$

where one has the direct sum decomposition

$$\operatorname{dom} \mathfrak{t}_{S_{K,0}} = \mathfrak{N}_0(T_{\max}) + \operatorname{dom} \mathfrak{t}_{A_{\mathrm{D}}} = \mathfrak{N}_0(T_{\max}) + H_0^1(\Omega),$$

and according to Lemma 8.5.2 $\{L^2(\partial\Omega), \Lambda\}$ is a boundary pair that is compatible with the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in Corollary 8.5.4.

In the nonnegative case a description of the nonnegative extensions and their form domains is of special interest. In the present situation Corollary 5.6.18 reads as follows.

Corollary 8.5.6. *Let $\Omega \subset \mathbb{R}^n$ be a bounded C^2-domain, let A_{D} be the self-adjoint Dirichlet realization of $-\Delta + V$ with $V \geq 0$, let $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ be the boundary triplet for $(T_{\min})^* = T_{\max}$ from Corollary 8.5.4, and let $\{L^2(\partial\Omega), \Lambda\}$ be the compatible boundary pair in (8.5.12). Then the formula*

$$\begin{aligned} \mathfrak{t}_{A_\Theta}[f,g] &= \mathfrak{t}_{S_{\mathrm{K},0}}[f,g] + \bigl(\Theta_{\mathrm{op}}^{\frac{1}{2}} \iota_- \widetilde{\tau}_{\mathrm{D}} f_0, \Theta_{\mathrm{op}}^{\frac{1}{2}} \iota_- \widetilde{\tau}_{\mathrm{D}} g_0\bigr)_{L^2(\partial\Omega)}, \\ \operatorname{dom} \mathfrak{t}_{A_\Theta} &= \bigl\{ f = f_0 + f_{\mathrm{F}} \in \operatorname{dom} \mathfrak{t}_{S_{\mathrm{K},0}} : \iota_- \widetilde{\tau}_{\mathrm{D}} f_0 \in \operatorname{dom} \Theta_{\mathrm{op}}^{\frac{1}{2}} \bigr\}, \end{aligned}$$

establishes a one-to-one correspondence between all closed nonnegative forms $\mathfrak{t}_{A_\Theta}$ corresponding to nonnegative self-adjoint extension A_Θ of $T_{\min}$ in $L^2(\Omega)$ and all closed nonnegative forms ω_Θ corresponding to nonnegative self-adjoint relations Θ in $L^2(\partial\Omega)$.

8.6 Coupling of Schrödinger operators

The aim of this section is to interpret the *natural* self-adjoint Schrödinger operator

$$A = -\Delta + V, \qquad \operatorname{dom} A = H^2(\mathbb{R}^n), \tag{8.6.1}$$

in $L^2(\mathbb{R}^n)$ with a real potential $V \in L^\infty(\mathbb{R}^n)$ as a coupling of Schrödinger operators on a bounded C^2-domain and its complement, that is, A is identified as a self-adjoint extension of the orthogonal sum of the minimal Schrödinger operators on the subdomains and its resolvent is expressed in a Kreĭn type resolvent formula. The present treatment is a multidimensional variant of the discussion in Section 6.5 and is based on the abstract coupling construction in Section 4.6.

Let $\Omega_+ \subset \mathbb{R}^n$ be a bounded C^2-domain and let $\Omega_- := \mathbb{R}^n \setminus \overline{\Omega}_+$ be the corresponding exterior domain. Since $\mathcal{C} := \partial\Omega_- = \partial\Omega_+$ is C^2-smooth in the sense of Definition 8.2.1, the term C^2-domain will be used here for Ω_-, although Ω_- is unbounded. In the following the common boundary $\mathcal{C}$ is sometimes referred to as an interface, linking the two domains Ω_+ and Ω_-. Note that one has the identification

$$L^2(\mathbb{R}^n) = L^2(\Omega_+) \oplus L^2(\Omega_-). \tag{8.6.2}$$

Consider the Schrödinger operator $A = -\Delta + V$, $\operatorname{dom} A = H^2(\mathbb{R}^n)$, in (8.6.1) with $V \in L^\infty(\mathbb{R}^n)$ real. Since the Laplacian $-\Delta$ defined on $H^2(\mathbb{R}^n)$ is unitarily equivalent in $L^2(\mathbb{R}^n)$ via the Fourier transform to the maximal multiplication operator with the function $x \mapsto |x|^2$, it is clear that $-\Delta$, and hence A in (8.6.1), is self-adjoint in $L^2(\mathbb{R}^n)$. Moreover, for $f \in C_0^\infty(\mathbb{R}^n)$ integration by parts shows that

$$(Af, f)_{L^2(\mathbb{R}^n)} = (\nabla f, \nabla f)_{L^2(\mathbb{R}^n;\mathbb{C}^n)} + (Vf, f)_{L^2(\mathbb{R}^n)} \geq v_- \|f\|^2_{L^2(\mathbb{R}^n)},$$

where $v_- = \operatorname{essinf} V$. As $C_0^\infty(\mathbb{R}^n)$ is dense in $H^2(\mathbb{R}^n)$, this estimate extends to $H^2(\mathbb{R}^n)$. Therefore, A is semibounded from below and v_- is a lower bound.

The restriction of the real function $V \in L^\infty(\Omega)$ to $\Omega_\pm$ is denoted by $V_\pm$ and the same $\pm$-index notation will be used for the restriction $f_\pm \in L^2(\Omega_\pm)$ of an element $f \in L^2(\mathbb{R}^n)$. The minimal and maximal operator associated with $-\Delta + V_+$ in $L^2(\Omega_+)$ will be denoted by $T^+_{\min}$ and $T^+_{\max}$, respectively, and the self-adjoint Dirichlet realization in $L^2(\Omega_+)$ will be denoted by A^+_{D}; cf. Proposition 8.3.1, Proposition 8.3.2, and Theorem 8.3.4. For the minimal operator

$$T^-_{\min} = -\Delta + V_-, \qquad \operatorname{dom} T^-_{\min} = H^2_0(\Omega_-),$$

and the maximal operator

$$\begin{aligned} T^-_{\max} &= -\Delta + V_-, \\ \operatorname{dom} T^-_{\max} &= \bigl\{ f_- \in L^2(\Omega_-) : -\Delta f_- + V_- f_- \in L^2(\Omega_-) \bigr\}, \end{aligned}$$

on the unbounded C^2-domain one can show in the same way as in the proof of Proposition 8.3.1 that $(T^-_{\min})^* = T^-_{\max}$ and $T^-_{\min} = (T^-_{\max})^*$. Furthermore, since Ω_- has a compact C^2-smooth boundary, it follows by analogy to Theorem 8.3.4 that the self-adjoint Dirichlet realization A^-_{D} corresponding to the densely defined closed semibounded form

$$\mathfrak{t}^-_{\mathrm{D}}[f_-, g_-] = (\nabla f_-, \nabla g_-)_{L^2(\Omega_-;\mathbb{C}^n)} + (V_- f_-, g_-)_{L^2(\Omega_-)}, \quad \operatorname{dom} \mathfrak{t}^-_{\mathrm{D}} = H^1_0(\Omega_-),$$

via the first representation theorem (Theorem 5.1.18) is given by

$$A^-_{\mathrm{D}} = -\Delta + V_-, \quad \operatorname{dom} A^-_{\mathrm{D}} = \bigl\{ f_- \in H^2(\Omega_-) : \tau^-_{\mathrm{D}} f_- = 0 \bigr\},$$

where τ^-_{D} denotes the Dirichlet trace operator on Ω_-; cf. (8.2.13). The operator A^-_{D} is semibounded from below and $v_- = \operatorname{essinf} V$ is a lower bound. In contrast to the Dirichlet operator A^+_{D}, the resolvent of A^-_{D} is not compact since Rellich's theorem is not valid on the unbounded domain Ω_-; cf. the proof of Proposition 8.3.2. Note also that the Dirichlet trace operator $\tau^-_{\mathrm{D}} : H^2(\Omega_-) \to H^{3/2}(\mathcal{C})$ and Neumann trace operator $\tau_{\rm N}^- : H^2(\Omega_-) \to H^{1/2}(\mathcal{C})$ have the same mapping properties as on a bounded domain. Moreover, both trace operators admit continuous extensions to $\operatorname{dom} T_{\max}^-$ as in Theorem 8.3.9 and Theorem 8.3.10. With the identification (8.6.2) it is clear that the orthogonal sum

$$\widetilde{A}_{\rm D} = \begin{pmatrix} A_{\rm D}^+ & 0 \\ 0 & A_{\rm D}^- \end{pmatrix} \tag{8.6.3}$$

is a self-adjoint operator in $L^2(\mathbb{R}^n)$ with Dirichlet boundary conditions on $\mathcal{C}$. The goal of the following considerations is to identify the self-adjoint Schrödinger operator A in (8.6.1) as a self-adjoint extension of the orthogonal sum of the minimal operators $T_{\min}^{\pm}$ and to compare A with the orthogonal sum $\widetilde{A}_{\rm D}$ in (8.6.3) using a Kreĭn type resolvent formula.

From now on it is assumed that $\eta < \operatorname{ess\,inf} V$ is fixed, so that, in particular, $\eta \in \rho(A_{\rm D}^+) \cap \rho(A_{\rm D}^-) \cap \mathbb{R}$. Consider the boundary triplet $\{L^2(\mathcal{C}), \Gamma_0^+, \Gamma_1^+\}$ for $T_{\max}^+$ in Theorem 8.4.1, that is,

$$\Gamma_0^+ f_+ = \iota_- \widetilde{\tau}_{\rm D}^+ f_+ \quad \text{and} \quad \Gamma_1^+ f_+ = -\iota_+ \tau_{\rm N}^+ f_{{\rm D},+}, \qquad f_+ \in \operatorname{dom} T_{\max}^+,$$

where $f_+ = f_{{\rm D},+} + f_{\eta,+}$ with $f_{{\rm D},+} \in \operatorname{dom} A_{\rm D}^+$ and $f_{\eta,+} \in \mathfrak{N}_\eta(T_{\max}^+)$. In the same way as in the proof of Theorem 8.4.1 one verifies that $\{L^2(\mathcal{C}), \Gamma_0^-, \Gamma_1^-\}$, where

$$\Gamma_0^- f_- = \iota_- \widetilde{\tau}_{\rm D}^- f_- \quad \text{and} \quad \Gamma_1^- f_- = -\iota_+ \tau_{\rm N}^- f_{{\rm D},-}, \qquad f_- \in \operatorname{dom} T_{\max}^-,$$

where $f_- = f_{{\rm D},-} + f_{\eta,-}$ with $f_{{\rm D},-} \in \operatorname{dom} A_{\rm D}^-$ and $f_{\eta,-} \in \mathfrak{N}_\eta(T_{\max}^-)$, is a boundary triplet for $T_{\max}^-$ such that $\operatorname{dom} A_{\rm D}^- = \ker \Gamma_0^-$. The γ-fields and Weyl functions in Proposition 8.4.4 corresponding to the boundary triplets $\{L^2(\mathcal{C}), \Gamma_0^\pm, \Gamma_1^\pm\}$ are denoted by $\gamma_\pm$ and $M_\pm$, respectively.

In analogy to Section 4.6, the orthogonal coupling of the boundary triplets $\{L^2(\mathcal{C}), \Gamma_0^+, \Gamma_1^+\}$ and $\{L^2(\mathcal{C}), \Gamma_0^-, \Gamma_1^-\}$ leads to the boundary triplet

$$\bigl\{L^2(\mathcal{C}) \oplus L^2(\mathcal{C}), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\bigr\} \tag{8.6.4}$$

for the orthogonal sum $T_{\max} := T_{\max}^+ \widehat{\oplus}\, T_{\max}^-$ of the maximal operator $T_{\max}^\pm$, where

$$\widetilde{\Gamma}_0 f = \begin{pmatrix} \Gamma_0^+ f_+ \\ \Gamma_0^- f_- \end{pmatrix} = \begin{pmatrix} \iota_- \widetilde{\tau}_{\rm D}^+ f_+ \\ \iota_- \widetilde{\tau}_{\rm D}^- f_- \end{pmatrix}, \quad f = \begin{pmatrix} f_+ \\ f_- \end{pmatrix}, \quad f_\pm \in \operatorname{dom} T_{\max}^\pm, \tag{8.6.5}$$

and

$$\widetilde{\Gamma}_1 f = \begin{pmatrix} \Gamma_1^+ f_+ \\ \Gamma_1^- f_- \end{pmatrix} = \begin{pmatrix} -\iota_+ \tau_{\rm N}^+ f_{{\rm D},+} \\ -\iota_+ \tau_{\rm N}^- f_{{\rm D},-} \end{pmatrix}, \quad f = \begin{pmatrix} f_+ \\ f_- \end{pmatrix}, \quad f_\pm \in \operatorname{dom} T_{\max}^\pm. \tag{8.6.6}$$

It is clear that

$$\operatorname{dom} A_{\rm D}^+ \times \operatorname{dom} A_{\rm D}^- = \ker \widetilde{\Gamma}_0,$$

and hence the self-adjoint operator in (8.6.3) coincides with the self-adjoint extension of $T_{\min} := T^+_{\min} \,\widehat{\oplus}\, T^-_{\min}$ corresponding to the boundary condition $\ker \widetilde{\Gamma}_0$. Note also that the corresponding γ-field $\widetilde{\gamma}$ and Weyl function $\widetilde{M}$ have the form

$$\widetilde{\gamma}(\lambda) = \begin{pmatrix} \gamma_+(\lambda) & 0 \\ 0 & \gamma_-(\lambda) \end{pmatrix} \quad \text{and} \quad \widetilde{M}(\lambda) = \begin{pmatrix} M_+(\lambda) & 0 \\ 0 & M_-(\lambda) \end{pmatrix} \tag{8.6.7}$$

for $\lambda \in \rho(A^+_{\mathrm{D}}) \cap \rho(A^-_{\mathrm{D}})$.

In Lemma 8.6.2 it will be shown that a certain relation $\widetilde{\Theta}$ is self-adjoint in $L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$. This relation will turn out to be the boundary parameter that corresponds to the Schrödinger operator A in (8.6.1) via the boundary triplet (8.6.4). The following lemma on the sum of the Dirichlet-to-Neumann maps is preparatory.

Lemma 8.6.1. *Let $\eta <$ essinf V and let $D_\pm(\lambda) : H^{3/2}(\mathcal{C}) \to H^{1/2}(\mathcal{C})$ be the Dirichlet-to-Neumann maps as in Definition 8.3.6 corresponding to $-\Delta + V_\pm$. Then for all $\lambda \in \mathbb{C} \setminus [\eta, \infty)$ the operator*

$$D_+(\lambda) + D_-(\lambda) : H^{3/2}(\mathcal{C}) \to H^{1/2}(\mathcal{C}) \tag{8.6.8}$$

is bijective.

Proof. First it will be shown that the operator in (8.6.8) is injective. Assume that $(D_+(\lambda) + D_-(\lambda))\varphi = 0$ for some $\varphi \in H^{3/2}(\mathcal{C})$ and some $\lambda \in \mathbb{C} \setminus [\eta, \infty)$. Then there exist $f_{\lambda,\pm} \in H^2(\Omega_\pm)$ such that

$$(-\Delta + V_\pm) f_{\lambda,\pm} = \lambda f_{\lambda,\pm}, \qquad \tau^+_{\mathrm{D}} f_{\lambda,+} = \tau^-_{\mathrm{D}} f_{\lambda,-} = \varphi, \tag{8.6.9}$$

and

$$0 = \bigl(D_+(\lambda) + D_-(\lambda)\bigr)\varphi = \bigl(D_+(\lambda) + D_-(\lambda)\bigr)\tau^\pm_{\mathrm{D}} f_{\lambda,\pm} = \tau^+_{\mathrm{N}} f_{\lambda,+} + \tau^-_{\mathrm{N}} f_{\lambda,-}.$$

As $\tau^+_{\mathrm{D}} f_{\lambda,+} = \tau^-_{\mathrm{D}} f_{\lambda,-}$ and $\tau^+_{\mathrm{N}} f_{\lambda,+} = -\tau^-_{\mathrm{N}} f_{\lambda,-}$ this implies that

$$f_\lambda = \begin{pmatrix} f_{\lambda,+} \\ f_{\lambda,-} \end{pmatrix} \in H^2(\mathbb{R}^n). \tag{8.6.10}$$

In fact, for each $h = (h_+, h_-)^\top \in \operatorname{dom} A = H^2(\mathbb{R}^n)$ one also has $\tau^+_{\mathrm{D}} h_+ = \tau^-_{\mathrm{D}} h_-$ and $\tau^+_{\mathrm{N}} h_+ = -\tau^-_{\mathrm{N}} h_-$ (note that the different signs are due to the fact that the Neumann trace on each domain is taken with respect to the outward normal vector) and hence

$$\begin{aligned}
(Ah, f_\lambda)_{L^2(\mathbb{R}^n)} &- (h, T_{\max} f_\lambda)_{L^2(\mathbb{R}^n)} \\
&= (T^+_{\max} h_+, f_{\lambda,+})_{L^2(\Omega_+)} - (h_+, T^+_{\max} f_{\lambda,+})_{L^2(\Omega_+)} \\
&\qquad + (T^-_{\max} h_-, f_{\lambda,-})_{L^2(\Omega_-)} - (h_-, T^-_{\max} f_{\lambda,-})_{L^2(\Omega_-)} \\
&= (\tau^+_{\mathrm{D}} h_+, \tau^+_{\mathrm{N}} f_{\lambda,+})_{L^2(\mathcal{C})} - (\tau^+_{\mathrm{N}} h_+, \tau^+_{\mathrm{D}} f_{\lambda,+})_{L^2(\mathcal{C})} \\
&\qquad + (\tau^-_{\mathrm{D}} h_-, \tau^-_{\mathrm{N}} f_{\lambda,-})_{L^2(\mathcal{C})} - (\tau^-_{\mathrm{N}} h_-, \tau^-_{\mathrm{D}} f_{\lambda,-})_{L^2(\mathcal{C})} \\
&= 0.
\end{aligned}$$

As the operator A is self-adjoint this shows, in particular, $f_\lambda \in \operatorname{dom} A$ and hence (8.6.10) holds. Furthermore, from (8.6.9) it follows that

$$Af_\lambda = (-\Delta + V)f_\lambda = \lambda f_\lambda.$$

Since $\sigma(A) \subset [v_-, \infty) \subset [\eta, \infty)$ and $\lambda \in \mathbb{C} \setminus [\eta, \infty)$, this implies that $f_\lambda = 0$ and hence $\varphi = \tau_D^\pm f_{\lambda,\pm} = 0$. Thus, it has been shown that the operator in (8.6.8) is injective for all $\lambda \in \mathbb{C} \setminus [\eta, \infty)$.

Next it will be shown that the operator in (8.6.8) is surjective. For this consider the space

$$H_{\mathcal{C}}(\mathbb{R}^n) := \left\{ f = \begin{pmatrix} f_+ \\ f_- \end{pmatrix} : f_\pm \in H^2(\Omega_\pm),\ \tau_D^+ f_+ = \tau_D^- f_- \right\}$$

and observe that as a consequence of (8.2.12) the mapping

$$\tau_N^{\mathcal{C}} : H_{\mathcal{C}}(\mathbb{R}^n) \to H^{1/2}(\mathcal{C}), \qquad f \mapsto \tau_N^{\mathcal{C}} f := \tau_N^+ f_+ + \tau_N^- f_-,$$

is surjective. For $\lambda \in \mathbb{C} \setminus [\eta, \infty)$ it will be shown now that the direct sum decomposition

$$H_{\mathcal{C}}(\mathbb{R}^n) = \operatorname{dom} A \dotplus \left\{ f_\lambda = \begin{pmatrix} f_{\lambda,+} \\ f_{\lambda,-} \end{pmatrix} : \begin{matrix} f_{\lambda,\pm} \in H^2(\Omega_\pm),\ \tau_D^+ f_{\lambda,+} = \tau_D^- f_{\lambda,-}, \\ (-\Delta + V_\pm) f_{\lambda,\pm} = \lambda f_{\lambda,\pm} \end{matrix} \right\}$$

holds. In fact, the inclusion ($\supset$) is clear since $\operatorname{dom} A = H^2(\mathbb{R}^n)$ and the second summand on the right-hand side is obviously contained in $H_{\mathcal{C}}(\mathbb{R}^n)$. The inclusion ($\subset$) follows from Theorem 1.7.1 applied to $T = -\Delta + V$, $\operatorname{dom} T = H_{\mathcal{C}}(\mathbb{R}^n)$, after observing that the space

$$\left\{ f_\lambda = \begin{pmatrix} f_{\lambda,+} \\ f_{\lambda,-} \end{pmatrix} : \begin{matrix} f_{\lambda,\pm} \in H^2(\Omega_\pm),\ \tau_D^+ f_{\lambda,+} = \tau_D^- f_{\lambda,-}, \\ (-\Delta + V_\pm) f_{\lambda,\pm} = \lambda f_{\lambda,\pm} \end{matrix} \right\} \tag{8.6.11}$$

coincides with $\mathfrak{N}_\lambda(T) = \ker(T - \lambda)$ and $\lambda \in \rho(A)$. Note also that $\lambda \in \rho(A)$ implies that the sum is direct.

Next observe that for $f \in \operatorname{dom} A$ one has $\tau_N^{\mathcal{C}} f = 0$ and hence also the restriction of $\tau_N^{\mathcal{C}}$ to the space (8.6.11) maps onto $H^{1/2}(\mathcal{C})$. Therefore, for $\psi \in H^{1/2}(\mathcal{C})$ there exists $f_\lambda = (f_{\lambda,+}, f_{\lambda,-})^\top$ such that $f_{\lambda,\pm} \in H^2(\Omega_\pm)$, $(-\Delta + V_\pm) f_{\lambda,\pm} = \lambda f_{\lambda,\pm}$,

$$\tau_D^+ f_{\lambda,+} = \tau_D^- f_{\lambda,-} =: \varphi \in H^{3/2}(\mathcal{C}) \quad \text{and} \quad \tau_N^{\mathcal{C}} f_\lambda = \tau_N^+ f_{\lambda,+} + \tau_N^- f_{\lambda,-} = \psi.$$

It follows that

$$\big(D_+(\lambda) + D_-(\lambda)\big)\varphi = D_+(\lambda)\tau_D^+ f_{\lambda,+} + D_-(\lambda)\tau_D^- f_{\lambda,-} = \tau_N^+ f_{\lambda,+} + \tau_N^- f_{\lambda,-} = \psi,$$

and hence the operator in (8.6.8) is surjective.

Consequently, it has been shown that (8.6.8) is a bijective operator for all $\lambda \in \mathbb{C} \setminus [\eta, \infty)$. □

Lemma 8.6.1 will be used to prove the following lemma on the self-adjointness of a particular relation $\widetilde{\Theta}$ in $L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$.

Lemma 8.6.2. *Let* $\eta < \operatorname{essinf} V$ *and let* $D_\pm(\eta) : H^{3/2}(\mathcal{C}) \to H^{1/2}(\mathcal{C})$ *be the Dirichlet-to-Neumann maps as in Definition 8.3.6 corresponding to* $-\Delta + V_\pm$*. Then the relation*

$$\widetilde{\Theta} = \left\{ \left\{ \begin{pmatrix} \xi \\ \xi \end{pmatrix}, \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \right\} : \xi \in H^2(\mathcal{C}),\ \varphi + \psi = \iota_+ \big(D_+(\eta) + D_-(\eta) \big) \iota_-^{-1} \xi \right\}$$

is self-adjoint in $L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$.

Proof. Recall first from Example 8.4.7 that $\iota_+ D_+(\eta) \iota_-^{-1}$ and $\iota_+ D_-(\eta) \iota_-^{-1}$ are both unbounded bijective self-adjoint operators in $L^2(\mathcal{C})$ with domain $H^2(\mathcal{C})$. Since $\eta < \operatorname{essinf} V$, one also sees from (8.4.18) that these operators are nonnegative. It follows, in particular, that $\iota_+ (D_+(\eta) + D_-(\eta)) \iota_-^{-1}$ is a symmetric operator in $L^2(\mathcal{C})$. Since

$$D_+(\eta) + D_-(\eta) : H^{3/2}(\mathcal{C}) \to H^{1/2}(\mathcal{C})$$

is bijective by Lemma 8.6.1 and the restricted operators $\iota_-^{-1} : H^2(\mathcal{C}) \to H^{3/2}(\mathcal{C})$ and $\iota_+ : H^{1/2}(\mathcal{C}) \to L^2(\mathcal{C})$ are also bijective, one concludes that

$$\iota_+ (D_+(\eta) + D_-(\eta)) \iota_-^{-1} \tag{8.6.12}$$

is a uniformly positive self-adjoint operator in $L^2(\mathcal{C})$ defined on $H^2(\mathcal{C})$.

To show that $\widetilde{\Theta} \subset \widetilde{\Theta}^*$, consider two arbitrary elements

$$\left\{ \begin{pmatrix} \xi \\ \xi \end{pmatrix}, \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \right\}, \left\{ \begin{pmatrix} \xi' \\ \xi' \end{pmatrix}, \begin{pmatrix} \varphi' \\ \psi' \end{pmatrix} \right\} \in \widetilde{\Theta},$$

that is, $\xi, \xi' \in H^2(\mathcal{C})$,

$$\varphi + \psi = \iota_+ \big(D_+(\eta) + D_-(\eta) \big) \iota_-^{-1} \xi \quad \text{and} \quad \varphi' + \psi' = \iota_+ \big(D_+(\eta) + D_-(\eta) \big) \iota_-^{-1} \xi'.$$

Then one computes

$$\begin{aligned}
&\left(\begin{pmatrix} \xi \\ \xi \end{pmatrix}, \begin{pmatrix} \varphi' \\ \psi' \end{pmatrix} \right)_{(L^2(\mathcal{C}))^2} - \left(\begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \begin{pmatrix} \xi' \\ \xi' \end{pmatrix} \right)_{(L^2(\mathcal{C}))^2} \\
&\quad = (\xi, \varphi' + \psi')_{L^2(\mathcal{C})} - (\varphi + \psi, \xi')_{L^2(\mathcal{C})} \\
&\quad = \big(\xi, \iota_+ \big(D_+(\eta) + D_-(\eta) \big) \iota_-^{-1} \xi' \big)_{L^2(\mathcal{C})} - \big(\iota_+ \big(D_+(\eta) + D_-(\eta) \big) \iota_-^{-1} \xi, \xi' \big)_{L^2(\mathcal{C})} \\
&\quad = 0,
\end{aligned}$$

where in the last step it was used that (8.6.12) is a symmetric operator in $L^2(\mathcal{C})$. Hence, the relation $\widetilde{\Theta}$ is symmetric in $L^2(\mathcal{C})$. For the opposite inclusion $\widetilde{\Theta}^* \subset \widetilde{\Theta}$ consider an element

$$\left\{ \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \begin{pmatrix} \gamma \\ \delta \end{pmatrix} \right\} \in \widetilde{\Theta}^*, \tag{8.6.13}$$

that is,

$$\left(\begin{pmatrix}\alpha\\ \beta\end{pmatrix}, \begin{pmatrix}\varphi\\ \psi\end{pmatrix}\right)_{(L^2(\mathcal{C}))^2} = \left(\begin{pmatrix}\gamma\\ \delta\end{pmatrix}, \begin{pmatrix}\xi\\ \xi\end{pmatrix}\right)_{(L^2(\mathcal{C}))^2} \tag{8.6.14}$$

holds for all

$$\left\{\begin{pmatrix}\xi\\ \xi\end{pmatrix}, \begin{pmatrix}\varphi\\ \psi\end{pmatrix}\right\} \in \widetilde{\Theta}.$$

The special choice $\xi = 0$ yields $\varphi + \psi = 0$ by the definition of $\widetilde{\Theta}$ and hence $(\alpha - \beta, \varphi)_{L^2(\mathcal{C})} = 0$ for all $\varphi \in L^2(\mathcal{C})$. This shows $\alpha = \beta$ and therefore (8.6.14) becomes

$$\big(\alpha, \iota_+\big(D_+(\eta) + D_-(\eta)\big)\iota_-^{-1}\xi\big)_{L^2(\mathcal{C})} = (\alpha, \varphi + \psi)_{L^2(\mathcal{C})} = (\gamma + \delta, \xi)_{L^2(\mathcal{C})}$$

for all $\xi \in H^2(\mathcal{C})$. Since $\iota_+(D_+(\eta) + D_-(\eta))\iota_-^{-1}$ is a self-adjoint operator in $L^2(\mathcal{C})$ defined on $H^2(\mathcal{C})$, it follows that $\alpha \in H^2(\mathcal{C})$ and

$$\iota_+\big(D_+(\eta) + D_-(\eta)\big)\iota_-^{-1}\alpha = \gamma + \delta.$$

This implies that the element in (8.6.13) belongs to $\widetilde{\Theta}$. Thus, $\widetilde{\Theta}$ is a self-adjoint relation in $L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$. □

The following theorem is the main result in this section. It turns out that the self-adjoint operator corresponding to $\widetilde{\Theta}$ in Lemma 8.6.2 coincides with the Schrödinger operator A.

Theorem 8.6.3. *Let $\{L^2(\mathcal{C}) \oplus L^2(\mathcal{C}), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ be the boundary triplet for $T_{\max}^+ \,\widehat{\oplus}\, T_{\max}^-$ from (8.6.4) with γ-field $\widetilde{\gamma}$, let $\widetilde{\Theta}$ be the self-adjoint relation in Lemma 8.6.2, and let $D_\pm(\lambda)$ be the Dirichlet-to-Neumann maps corresponding to $-\Delta + V_\pm$. Then the self-adjoint operator $\widetilde{A}_{\widetilde{\Theta}}$ corresponding to the parameter $\widetilde{\Theta}$ coincides with the Schrödinger operator A in (8.6.1) and for all $\lambda \in \mathbb{C} \setminus [\eta, \infty)$ one has the resolvent formula*

$$(A - \lambda)^{-1} = (\widetilde{A}_{\mathrm{D}} - \lambda)^{-1} + \widetilde{\gamma}(\lambda)\widetilde{\Lambda}(\lambda)\widetilde{\gamma}(\bar{\lambda})^*,$$

where $\widetilde{\Lambda}(\lambda) \in \mathbf{B}(L^2(\mathcal{C}) \oplus L^2(\mathcal{C}))$ has the form

$$\widetilde{\Lambda}(\lambda) = \begin{pmatrix} \iota_-(D_+(\lambda) + D_-(\lambda))^{-1}\iota_+^{-1} & \iota_-(D_+(\lambda) + D_-(\lambda))^{-1}\iota_+^{-1} \\ \iota_-(D_+(\lambda) + D_-(\lambda))^{-1}\iota_+^{-1} & \iota_-(D_+(\lambda) + D_-(\lambda))^{-1}\iota_+^{-1} \end{pmatrix}.$$

Proof. First it will be shown that the self-adjoint extension $\widetilde{A}_{\widetilde{\Theta}}$ and the self-adjoint Schrödinger operator A in (8.6.1) coincide. Since both operators are self-adjoint, it suffices to verify the inclusion $A \subset \widetilde{A}_{\widetilde{\Theta}}$. For this, consider $f \in \operatorname{dom} A = H^2(\mathbb{R}^n)$ and note that $f = (f_+, f_-)^\top$ satisfies $\tau_{\mathrm{D}}^+ f_+ = \tau_{\mathrm{D}}^- f_-$ and $\tau_{\mathrm{N}}^+ f_+ = -\tau_{\mathrm{N}}^- f_-$. It will be shown that $\{\widetilde{\Gamma}_0 f, \widetilde{\Gamma}_1 f\} \in \widetilde{\Theta}$. By the definition of the boundary mappings $\widetilde{\Gamma}_0$ and $\widetilde{\Gamma}_1$ in (8.6.5)–(8.6.6), one has

$$\widetilde{\Gamma}_0 f = \begin{pmatrix} \iota_-\widetilde{\tau}_{\mathrm{D}}^+ f_+ \\ \iota_-\widetilde{\tau}_{\mathrm{D}}^- f_- \end{pmatrix} \quad \text{and} \quad \widetilde{\Gamma}_1 f = \begin{pmatrix} -\iota_+\tau_{\mathrm{N}}^+ f_{\mathrm{D},+} \\ -\iota_+\tau_{\mathrm{N}}^- f_{\mathrm{D},-} \end{pmatrix} =: \begin{pmatrix} \varphi \\ \psi \end{pmatrix}$$

and, as $f \in H^2(\mathbb{R}^n)$, it follows that

$$\xi := \iota_- \tau_D^+ f_+ = \iota_- \widetilde{\tau}_D^+ f_+ = \iota_- \widetilde{\tau}_D^- f_- = \iota_- \tau_D^- f_- \in H^2(\mathcal{C}).$$

Since $f_\pm = f_{D,\pm} + f_{\eta,\pm}$ with $f_{D,\pm} \in \operatorname{dom} A_D^\pm$ and $f_{\eta,\pm} \in \mathfrak{N}_\eta(T_{\max}^\pm)$, one has $\tau_D^\pm f_\pm = \tau_D^\pm f_{\eta,\pm}$ and one concludes that

$$\begin{aligned}
\iota_+\bigl(D_+(\eta) + D_-(\eta)\bigr)\iota_-^{-1}\xi &= \iota_+\bigl(D_+(\eta)\tau_D^+ f_{\eta,+} + D_-(\eta)\tau_D^- f_{\eta,-}\bigr) \\
&= \iota_+\bigl(\tau_N^+ f_{\eta,+} + \tau_N^- f_{\eta,-}\bigr) \\
&= \iota_+\bigl(\tau_N^+ f_+ + \tau_N^- f_- - \tau_N^+ f_{D,+} - \tau_N^- f_{D,-}\bigr) \\
&= -\iota_+\tau_N^+ f_{D,+} - \iota_+\tau_N^- f_{D,-} \\
&= \varphi + \psi,
\end{aligned}$$

where the property $\tau_N^+ f_+ = -\tau_N^- f_-$ for $f \in \operatorname{dom} A$ was used. These considerations imply $\{\widetilde{\Gamma}_0 f, \widetilde{\Gamma}_1 f\} \in \widetilde{\Theta}$ and thus $f \in \operatorname{dom} \widetilde{A}_{\widetilde{\Theta}}$. Therefore, $\operatorname{dom} A = H^2(\mathbb{R}^n)$ is contained in $\operatorname{dom} \widetilde{A}_{\widetilde{\Theta}}$, and since both operators are self-adjoint, it follows that they coincide, that is, $A = \widetilde{A}_{\widetilde{\Theta}}$.

As a consequence of Theorem 2.6.1 one has for $\lambda \in \rho(A) \cap \rho(\widetilde{A}_D)$ that

$$(A-\lambda)^{-1} = (\widetilde{A}_D - \lambda)^{-1} + \widetilde{\gamma}(\lambda)\bigl(\widetilde{\Theta} - \widetilde{M}(\lambda)\bigr)^{-1}\widetilde{\gamma}(\bar{\lambda})^*,$$

where $\widetilde{\gamma}$ and $\widetilde{M}$ are the γ-field and Weyl function, respectively, of the boundary triplet $\{L^2(\mathcal{C}) \oplus L^2(\mathcal{C}), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ in (8.6.7). Here it is also clear from Theorem 2.6.1 that

$$\bigl(\widetilde{\Theta} - \widetilde{M}(\lambda)\bigr)^{-1} \in \mathbf{B}(L^2(\mathcal{C}) \oplus L^2(\mathcal{C})), \qquad \lambda \in \rho(A) \cap \rho(\widetilde{A}_D).$$

From now consider only $\lambda \in \mathbb{C} \setminus [\eta, \infty)$. It follows from Lemma 8.6.2 and (8.6.7) that

$$\begin{aligned}
&\bigl(\widetilde{\Theta} - \widetilde{M}(\lambda)\bigr)^{-1} \\
&= \left\{ \left\{ \begin{pmatrix} \varphi - M_+(\lambda)\xi \\ \psi - M_-(\lambda)\xi \end{pmatrix}, \begin{pmatrix} \xi \\ \xi \end{pmatrix} \right\} : \begin{matrix} \xi \in H^2(\mathcal{C}), \\ \varphi + \psi = \iota_+\bigl(D_+(\eta) + D_-(\eta)\bigr)\iota_-^{-1}\xi \end{matrix} \right\},
\end{aligned}$$

and setting $\vartheta_1 = \varphi - M_+(\lambda)\xi$ and $\vartheta_2 = \psi - M_-(\lambda)\xi$ one obtains

$$\begin{aligned}
\vartheta_1 + \vartheta_2 &= \varphi + \psi - M_+(\lambda)\xi - M_-(\lambda)\xi \\
&= \iota_+\bigl(D_+(\eta) + D_-(\eta)\bigr)\iota_-^{-1}\xi - M_+(\lambda)\xi - M_-(\lambda)\xi.
\end{aligned}$$

Since $M_\pm(\lambda)\xi = \iota_+(D_\pm(\eta) - D_\pm(\lambda))\iota_-^{-1}\xi$ for $\xi \in H^2(\mathcal{C})$ by Lemma 8.4.5, it follows that

$$\vartheta_1 + \vartheta_2 = \iota_+\bigl(D_+(\lambda) + D_-(\lambda)\bigr)\iota_-^{-1}\xi.$$

Lemma 8.6.1 implies that $\iota_+(D_+(\lambda) + D_-(\lambda))\iota_-^{-1}$ is a bijective operator in $L^2(\mathcal{C})$ for $\lambda \in \mathbb{C} \setminus [\eta, \infty)$ and hence

$$\iota_-\bigl(D_+(\lambda) + D_-(\lambda)\bigr)^{-1}\iota_+^{-1}\vartheta_1 + \iota_-\bigl(D_+(\lambda) + D_-(\lambda)\bigr)^{-1}\iota_+^{-1}\vartheta_2 = \xi.$$

Therefore, one has

$$\big(\widetilde{\Theta} - \widetilde{M}(\lambda)\big)^{-1} = \begin{pmatrix} \iota_-(D_+(\lambda)+D_-(\lambda))^{-1}\iota_+^{-1} & \iota_-(D_+(\lambda)+D_-(\lambda))^{-1}\iota_+^{-1} \\ \iota_-(D_+(\lambda)+D_-(\lambda))^{-1}\iota_+^{-1} & \iota_-(D_+(\lambda)+D_-(\lambda))^{-1}\iota_+^{-1} \end{pmatrix}.$$

This completes the proof of Theorem 8.6.3. □

Finally, the boundary triplet in (8.6.4) is modified in the same way as in Proposition 4.6.4 to interpret the Schrödinger operator A as the self-adjoint extension corresponding to the boundary mapping $\widehat{\Gamma}_0$. More precisely, the boundary triplets $\{L^2(\mathcal{C}), \Gamma_0^+, \Gamma_1^+\}$ and $\{L^2(\mathcal{C}), \Gamma_0^-, \Gamma_1^-\}$ lead to the boundary triplet

$$\big\{L^2(\mathcal{C}) \oplus L^2(\mathcal{C}), \widehat{\Gamma}_0, \widehat{\Gamma}_1\big\} \tag{8.6.15}$$

for $T_{\max} = T_{\max}^+ \mathbin{\widehat{\oplus}} T_{\max}^-$, where

$$\widehat{\Gamma}_0 f = \begin{pmatrix} -\Gamma_1^+ f_+ - \Gamma_1^- f_- \\ \Gamma_0^+ f_+ - \Gamma_0^- f_- \end{pmatrix} = \begin{pmatrix} \iota_+(\tau_N^+ f_{D,+} + \tau_N^- f_{D,-}) \\ \iota_-(\widetilde{\tau}_D^+ f_+ - \widetilde{\tau}_D^- f_-) \end{pmatrix}$$

and

$$\widehat{\Gamma}_1 f = \begin{pmatrix} \Gamma_0^+ f_+ \\ -\Gamma_1^- f_- \end{pmatrix} = \begin{pmatrix} \iota_- \widetilde{\tau}_D^+ f_+ \\ \iota_+ \tau_N^- f_{D,-} \end{pmatrix}$$

for $f = (f_+, f_-)^\top$ with $f_\pm \in \operatorname{dom} T_{\max}^\pm$. It follows from Proposition 4.6.4 that the Schrödinger operator $A = -\Delta + V$ in (8.6.1) coincides with the self-adjoint extension defined on $\ker \widehat{\Gamma}_0$ and that the Weyl function corresponding to the boundary triplet in (8.6.15) is given by

$$\widehat{M}(\lambda) = -\begin{pmatrix} M_+(\lambda) & -I \\ -I & -M_-(\lambda)^{-1} \end{pmatrix}^{-1}, \qquad \lambda \in \mathbb{C} \setminus \mathbb{R},$$

where $M_\pm(\lambda) = \iota_+(\widetilde{D}_\pm(\eta) - \widetilde{D}_\pm(\lambda))\iota_-^{-1}$ is the Weyl function corresponding to the boundary triplet $\{L^2(\mathcal{C}), \Gamma_0^\pm, \Gamma_1^\pm\}$; cf. Proposition 8.4.4 and Lemma 8.4.5. In particular, the results in Section 3.5 and Section 3.6 can be used to describe the isolated and embedded eigenvalues, continuous, and absolutely continuous spectrum of A with the help of the limit properties of the Dirichlet-to-Neumann maps $\widetilde{D}_\pm$. For this, however, one has to ensure that the underlying minimal operator $T_{\min} = T_{\min}^+ \mathbin{\widehat{\oplus}} T_{\min}^-$ is simple, which follows from Proposition 8.3.13 and [120, Proposition 2.2].

8.7 Bounded Lipschitz domains

In this last section Schrödinger operators $-\Delta + V$ with a real function $V \in L^\infty(\Omega)$ on bounded Lipschitz domains are briefly discussed. This situation is more general than the setting of bounded C^2-domains treated in the previous sections. The main objective here is to highlight the differences to the C^2-case and to indicate which methods have to be adapted in order to obtain results of similar nature as above.

The notions of a Lipschitz hypograph and a bounded Lipschitz domain are defined in the same way as C^2-hypographs and bounded C^2-domains in Section 8.2. More precisely, for a Lipschitz continuous function $\phi : \mathbb{R}^{n-1} \to \mathbb{R}$ the domain

$$\Omega_\phi := \{(x', x_n)^\top \in \mathbb{R}^n : x_n < \phi(x')\}$$

is called a *Lipschitz hypograph* with boundary $\partial\Omega$. The surface integral and surface measure on $\partial\Omega_\phi$ are defined in the same way as in (8.2.4), and this leads to the L^2-space $L^2(\partial\Omega_\phi)$ on $\partial\Omega_\phi$. For $s \in [0,1]$ define the Sobolev space of order s on $\partial\Omega_\phi$ by

$$H^s(\partial\Omega_\phi) := \{h \in L^2(\partial\Omega_\phi) : x' \mapsto h(x', \phi(x')) \in H^s(\mathbb{R}^{n-1})\}$$

and equip $H^s(\partial\Omega_\phi)$ with the corresponding scalar product (8.2.6).

Definition 8.7.1. A bounded nonempty open subset $\Omega \subset \mathbb{R}^n$ is called a *Lipschitz domain* if there exist open sets $U_1, \dots, U_l \subset \mathbb{R}^n$ and (possibly up to rotations of coordinates) Lipschitz hypographs $\Omega_1, \dots, \Omega_l \subset \mathbb{R}^n$, such that

$$\partial\Omega \subset \bigcup_{j=1}^{l} U_j \quad \text{and} \quad \Omega \cap U_j = \Omega_j \cap U_j, \quad j = 1, \dots, l.$$

For a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$ the boundary $\partial\Omega \subset \mathbb{R}^n$ is compact. Using a partition of unity subordinate to the open cover $\{U_j\}$ of $\partial\Omega$ one defines the surface integral, surface measure, and the L^2-space $L^2(\partial\Omega)$ in the same way as in Section 8.2. The Sobolev space $H^s(\partial\Omega)$ for $s \in [0,1]$ is then defined by

$$H^s(\partial\Omega) := \{h \in L^2(\partial\Omega) : \eta_j h \in H^s(\partial\Omega_j),\ j = 1, \dots, l\}$$

and equipped with the corresponding Hilbert space scalar product (8.2.7). It follows that $H^s(\partial\Omega)$, $s \in [0,1]$, is densely and continuously embedded in $L^2(\partial\Omega)$, and the embedding $H^t(\partial\Omega) \hookrightarrow H^s(\partial\Omega)$ is compact for $s < t \le 1$. As in Section 8.2, the spaces $H^s(\partial\Omega)$, $s \in [0,1]$, can be defined in an equivalent way via interpolation. The dual space of the antilinear continuous functionals on $H^s(\partial\Omega)$ is denoted by $H^{-s}(\partial\Omega)$, $s \in [0,1]$.

For a bounded Lipschitz domain Ω define the spaces

$$H^s_\Delta(\Omega) := \{f \in H^s(\Omega) : \Delta f \in L^2(\Omega)\}, \qquad s \ge 0,$$

and equip them with the Hilbert space scalar product

$$(f,g)_{H^s_\Delta(\Omega)} := (f,g)_{H^s(\Omega)} + (\Delta f, \Delta g)_{L^2(\Omega)}, \qquad f,g \in H^s_\Delta(\Omega). \tag{8.7.1}$$

It is clear that $H^s(\Omega) = H^s_\Delta(\Omega)$ for $s \ge 2$ and that $H^0_\Delta(\Omega) = \operatorname{dom} T_{\max}$ for $s = 0$, with (8.7.1) as the graph norm; cf. (8.3.3). The unit normal vector field pointing outwards on $\partial\Omega$ will again be denoted by ν. It is known that the Dirichlet trace mapping $C^\infty(\overline{\Omega}) \ni f \mapsto f|_{\partial\Omega}$ extends by continuity to a continuous surjective mapping

$$\tau_{\mathrm{D}} : H^s_\Delta(\Omega) \to H^{s-1/2}(\partial\Omega), \qquad \frac{1}{2} \leq s \leq \frac{3}{2},$$

and that the Neumann trace mapping $C^\infty(\overline{\Omega}) \ni f \mapsto \nu \cdot \nabla f|_{\partial\Omega}$ extends by continuity to a continuous surjective mapping

$$\tau_{\mathrm{N}} : H^s_\Delta(\Omega) \to H^{s-3/2}(\partial\Omega), \qquad \frac{1}{2} \leq s \leq \frac{3}{2};$$

cf. [92, 326]. For the present purposes it is particularly useful to note that the mappings

$$\tau_{\mathrm{D}} : H^{3/2}_\Delta(\Omega) \to H^1(\partial\Omega) \quad \text{and} \quad \tau_{\mathrm{N}} : H^{3/2}_\Delta(\Omega) \to L^2(\partial\Omega) \tag{8.7.2}$$

are both continuous and surjective. Furthermore, the first and second Green identities remain true in the natural form, that is,

$$(-\Delta f, g)_{L^2(\Omega)} = (\nabla f, \nabla g)_{L^2(\Omega;\mathbb{C}^n)} - \big\langle \tau_{\mathrm{N}} f, \tau_{\mathrm{D}} g \big\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)}$$

and

$$\begin{aligned}(-\Delta f, g)_{L^2(\Omega)} &- (f, -\Delta g)_{L^2(\Omega)} \\ &= \big\langle \tau_{\mathrm{D}} f, \tau_{\mathrm{N}} g \big\rangle_{H^{1/2}(\partial\Omega)\times H^{-1/2}(\partial\Omega)} - \big\langle \tau_{\mathrm{N}} f, \tau_{\mathrm{D}} g \big\rangle_{H^{-1/2}(\partial\Omega)\times H^{1/2}(\partial\Omega)}\end{aligned}$$

hold for all $f, g \in H^1_\Delta(\Omega)$.

The minimal operator $T_{\min}$ and maximal operator $T_{\max}$ associated with $-\Delta + V$ on a bounded Lipschitz domain are defined in exactly the same way as in the beginning of Section 8.3. The assertions $T^*_{\min} = T_{\max}$ and $T_{\min} = T^*_{\max}$ in Proposition 8.3.1 remain valid in the present situation. Furthermore, the Dirichlet realization A_{D} and Neumann realization A_{N} of $-\Delta + V$ are defined as in Section 8.3, and their properties are the same as in Proposition 8.3.2 and Proposition 8.3.3. The first remarkable and substantial difference for Schrödinger operators on a bounded Lipschitz domain appears in connection with the regularity of the domains of A_{D} and A_{N} when comparing with Theorem 8.3.4. In the present case one has the following regularity result from [431, 432], see also [92, 323].

Theorem 8.7.2. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain. Then one has*

$$A_{\mathrm{D}} f = -\Delta f + V f, \quad \operatorname{dom} A_{\mathrm{D}} = \big\{ f \in H^{3/2}_\Delta(\Omega) : \tau_{\mathrm{D}} f = 0 \big\},$$

and

$$A_{\mathrm{N}} f = -\Delta f + V f, \quad \operatorname{dom} A_{\mathrm{N}} = \big\{ f \in H^{3/2}_\Delta(\Omega) : \tau_{\mathrm{N}} f = 0 \big\}.$$

The same reasoning as in Section 8.3 one obtains the following useful decomposition of the space $H^{3/2}_\Delta(\Omega)$.

Corollary 8.7.3. *Assume that* $\Omega \subset \mathbb{R}^n$ *is a bounded Lipschitz domain. Then for* $\lambda \in \rho(A_{\rm D})$ *one has the direct sum decomposition*

$$\begin{aligned} H^{3/2}_\Delta(\Omega) &= \operatorname{dom} A_{\rm D} \dotplus \bigl\{ f_\lambda \in H^{3/2}_\Delta(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\} \\ &= \ker \tau_{\rm D} \dotplus \bigl\{ f_\lambda \in H^{3/2}_\Delta(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\}, \end{aligned}$$

and for $\lambda \in \rho(A_{\rm N})$ *one has the direct sum decomposition*

$$\begin{aligned} H^{3/2}_\Delta(\Omega) &= \operatorname{dom} A_{\rm N} \dotplus \bigl\{ f_\lambda \in H^{3/2}_\Delta(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\} \\ &= \ker \tau_{\rm N} \dotplus \bigl\{ f_\lambda \in H^{3/2}_\Delta(\Omega) : (-\Delta + V) f_\lambda = \lambda f_\lambda \bigr\}. \end{aligned}$$

For a bounded Lipschitz domain and $\lambda \in \rho(A_{\rm D})$ the Dirichlet-to-Neumann map is defined as

$$D(\lambda) : H^1(\partial\Omega) \to L^2(\partial\Omega), \qquad \tau_{\rm D} f_\lambda \mapsto \tau_{\rm N} f_\lambda, \tag{8.7.3}$$

where $f_\lambda \in H^{3/2}_\Delta(\Omega)$ is such that $(-\Delta + V) f_\lambda = \lambda f_\lambda$. This definition is the natural analog of Definition 8.3.6, taking into account the decomposiion in (8.7.3). As before, it follows that for $\lambda \in \rho(A_{\rm D}) \cap \rho(A_{\rm N})$ the Dirichlet-to-Neumann map (8.7.3) is a bijective operator.

For completeness the following a priori estimates are stated.

Corollary 8.7.4. *Assume that* $\Omega \subset \mathbb{R}^n$ *is a bounded Lipschitz domain. Then there exist constants* $C_{\rm D} > 0$ *and* $C_{\rm N} > 0$ *such that*

$$\|f\|_{H^{3/2}_\Delta(\Omega)} \leq C_{\rm D} \bigl(\|f\|_{L^2(\Omega)} + \|A_{\rm D} f\|_{L^2(\Omega)} \bigr), \quad f \in \operatorname{dom} A_{\rm D},$$

and

$$\|g\|_{H^{3/2}_\Delta(\Omega)} \leq C_{\rm N} \bigl(\|g\|_{L^2(\Omega)} + \|A_{\rm N} g\|_{L^2(\Omega)} \bigr) \quad g \in \operatorname{dom} A_{\rm N}.$$

Next a variant of Theorem 8.3.9 and Theorem 8.3.10 on the extensions of the Dirichlet and Neumann trace operators to $\operatorname{dom} T_{\max} = H^0_\Delta(\Omega)$ for bounded Lipschitz domains is formulated. For this consider the spaces

$$\mathscr{G}_0 := \bigl\{ \tau_{\rm D} f : f \in \operatorname{dom} A_{\rm N} \bigr\} \quad \text{and} \quad \mathscr{G}_1 := \bigl\{ \tau_{\rm N} g : g \in \operatorname{dom} A_{\rm D} \bigr\}, \tag{8.7.4}$$

and note that for the special case of a bounded C^2-domain the spaces $\mathscr{G}_0$ and $\mathscr{G}_1$ coincide with the spaces $H^{3/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega)$, respectively. The spaces $\mathscr{G}_0$ and $\mathscr{G}_1$ are dense in $L^2(\partial\Omega)$ and, equipped with the scalar products

$$\begin{aligned} (\varphi, \psi)_{\mathscr{G}_0} &:= (\Sigma^{-1/2} \varphi, \Sigma^{-1/2} \psi)_{L^2(\partial\Omega)}, \qquad &\Sigma = \operatorname{Im}\,(D(i)^{-1}), \\ (\varphi, \psi)_{\mathscr{G}_1} &:= (\Lambda^{-1/2} \varphi, \Lambda^{-1/2} \psi)_{L^2(\partial\Omega)}, \qquad &\Lambda = -\overline{\operatorname{Im} D(i)}, \end{aligned} \tag{8.7.5}$$

they are Hilbert spaces, as was shown in [92, 115]; here both $\Sigma^{-1/2}$ and $\Lambda^{-1/2}$ are unbounded nonnegative self-adjoint operators in $L^2(\partial\Omega)$. The corresponding dual spaces of antilinear continuous functionals are denoted by $\mathscr{G}_0'$ and $\mathscr{G}_1'$, respectively, and one obtains Gelfand triples $\{\mathscr{G}_i, L^2(\partial\Omega), \mathscr{G}_i'\}$, $i = 0, 1$, which serve as the counterparts of $\{H^s(\partial\Omega), L^2(\partial\Omega), H^s(\partial\Omega)\}$, $s = 1/2, 3/2$. Now one can prove the variant of Theorem 8.3.9 and Theorem 8.3.10 alluded to above.

Theorem 8.7.5. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain. Then the Dirichlet and Neumann trace operators in (8.7.2) admit unique extensions to continuous surjective operators*

$$\widetilde{\tau}_{\mathrm{D}} : \operatorname{dom} T_{\max} \to \mathscr{G}_1' \quad \textit{and} \quad \widetilde{\tau}_{\mathrm{N}} : \operatorname{dom} T_{\max} \to \mathscr{G}_0',$$

where $\operatorname{dom} T_{\max}$ *is equipped with the graph norm. Furthermore,*

$$\ker \widetilde{\tau}_{\mathrm{D}} = \ker \tau_{\mathrm{D}} = \operatorname{dom} A_{\mathrm{D}} \quad \textit{and} \quad \ker \widetilde{\tau}_{\mathrm{N}} = \ker \tau_{\mathrm{N}} = \operatorname{dom} A_{\mathrm{N}}.$$

By analogy to Corollary 8.3.11, the second Green identity extends to elements $f \in \operatorname{dom} T_{\max}$ and $g \in \operatorname{dom} A_{\mathrm{D}}$ in the form

$$(T_{\max} f, g)_{L^2(\Omega)} - (f, T_{\max} g)_{L^2(\Omega)} = \langle \widetilde{\tau}_{\mathrm{D}} f, \tau_{\mathrm{N}} g \rangle_{\mathscr{G}_1' \times \mathscr{G}_1},$$

and for $f \in \operatorname{dom} T_{\max}$ and $g \in \operatorname{dom} A_{\mathrm{N}}$ the second Green identity reads

$$(T_{\max} f, g)_{L^2(\Omega)} - (f, T_{\max} g)_{L^2(\Omega)} = -\langle \widetilde{\tau}_{\mathrm{N}} f, \tau_{\mathrm{D}} g \rangle_{\mathscr{G}_0' \times \mathscr{G}_0}.$$

It will also be used that for $\lambda \in \rho(A_{\mathrm{D}})$ the Dirichlet-to-Neumann map in (8.7.3) admits an extension to a bounded operator

$$\widetilde{D}(\lambda) : \mathscr{G}_1' \to \mathscr{G}_0', \qquad \widetilde{\tau}_{\mathrm{D}} f_\lambda \mapsto \widetilde{\tau}_{\mathrm{N}} f_\lambda, \tag{8.7.6}$$

where $f_\lambda \in \mathfrak{N}_\lambda(T_{\max})$.

With the preparations above one can now follow the strategy in Section 8.4 and construct a boundary triplet for the maximal operator $T_{\max}$ under the assumption that $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain. Consider the Gelfand triple $\{\mathscr{G}_1, L^2(\partial\Omega), \mathscr{G}_1'\}$ and the corresponding isometric isomorphisms $\iota_+ : \mathscr{G}_1 \to L^2(\partial\Omega)$ and $\iota_- : \mathscr{G}_1' \to L^2(\partial\Omega)$ such that

$$\langle \varphi, \psi \rangle_{\mathscr{G}_1' \times \mathscr{G}_1} = (\iota_- \varphi, \iota_+ \psi)_{L^2(\partial\Omega)}, \qquad \varphi \in \mathscr{G}_1',\ \psi \in \mathscr{G}_1;$$

cf. Lemma 8.1.2. When comparing (8.1.6) and (8.7.5) it is clear that $\iota_+ = \Lambda^{-1/2}$ and ι_- is the extension of $\Lambda^{1/2}$ onto $\mathscr{G}_1'$. Recall also the definition and the properties of the Dirichlet operator A_{D} in Theorem 8.7.2 and the direct sum decomposition (8.4.1).

Theorem 8.7.6. *Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain and let A_{D} be the self-adjoint Dirichlet realization of $-\Delta + V$ in $L^2(\Omega)$ in Theorem 8.7.2. Fix a number $\eta \in \rho(A_{\mathrm{D}}) \cap \mathbb{R}$ and decompose $f \in \operatorname{dom} T_{\max}$ according to (8.4.1) in the form*

$f = f_{\rm D} + f_\eta$, *where* $f_{\rm D} \in \operatorname{dom} A_{\rm D}$ *and* $f_\eta \in \mathfrak{N}_\eta(T_{\max})$. *Then* $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$, *where*

$$\Gamma_0 f = \iota_- \widetilde{\tau}_{\rm D} f \quad \textit{and} \quad \Gamma_1 f = -\iota_+ \tau_{\rm N} f_{\rm D}, \qquad f = f_{\rm D} + f_\eta \in \operatorname{dom} T_{\max},$$

is a boundary triplet for $(T_{\min})^* = T_{\max}$ *such that*

$$A_0 = A_{\rm D} \qquad \textit{and} \qquad A_1 = T_{\min} \,\widehat{+}\, \widehat{\mathfrak{N}}_\eta(T_{\max}).$$

The γ-field and Weyl function corresponding to the boundary triplet in Theorem 8.7.6 are formally the same as in Proposition 8.4.4. In fact, if $f_\eta(\varphi)$ denotes the unique element in $\mathfrak{N}_\eta(T_{\max})$ such that $\Gamma_0 f_\eta(\varphi) = \varphi$, then for all $\lambda \in \rho(A_{\rm D})$ the γ-field is given by

$$\gamma(\lambda)\varphi = \bigl(I + (\lambda - \eta)(A_{\rm D} - \lambda)^{-1}\bigr) f_\eta(\varphi), \quad \varphi \in L^2(\partial\Omega),$$

where $f_\lambda(\varphi) := \gamma(\lambda)\varphi$ is the unique element in $\mathfrak{N}_\lambda(T_{\max})$ such that $\Gamma_0 f_\lambda(\varphi) = \varphi$. As in Proposition 8.4.4 one also has

$$\gamma(\lambda)^* = -\iota_+ \tau_{\rm N} (A_{\rm D} - \bar{\lambda})^{-1}, \quad \lambda \in \rho(A_{\rm D}).$$

Moreover, the Weyl function M is given by

$$M(\lambda)\varphi = (\eta - \lambda)\iota_+ \tau_{\rm N} (A_{\rm D} - \lambda)^{-1} f_\eta(\varphi), \quad \varphi \in L^2(\partial\Omega).$$

As in the case of bounded C^2-domains, the Weyl function can be expressed via the Dirichlet-to-Neumann map; here the extended mapping $\widetilde{D}(\lambda)$ in (8.7.6) is used. In the same way as in Lemma 8.4.5 one verifies the relation

$$M(\lambda) = \iota_+ \bigl(\widetilde{D}(\eta) - \widetilde{D}(\lambda)\bigr)\iota_-^{-1}.$$

With the boundary triplet $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in Theorem 8.7.6 and the corresponding γ-field and Weyl function the self-adjoint realizations of $-\Delta + V$ on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$ can be parametrized and the spectral properties can be described in a similar form as in Section 8.4. The discussion of the semibounded extensions and of the corresponding sesquilinear forms with the help of a compatible boundary pair is parallel to the considerations in Section 8.5 and is not provided here. Finally, the coupling technique of Schrödinger operators from Section 8.6 also extends under appropriate modifications to the general situation of Lipschitz domains.