# Chapter 7

# Boundary Triples and Self-Adjointness

A simple variation of the not so popular approach to self-adjoint extensions via boundary triples is discussed. The idea is exemplified through a series of examples, including the one-dimensional hydrogen atom, free hamiltonian in an interval and spherically symmetric potentials. At the end, important self-adjoint extensions of a quantum particle hamiltonian in a multiply connected domain are found.

## 7.1 Boundary Forms

If $T \subset S$ are hermitian operators one has $T \subset S \subset S^* \subset T^*$, that is, any hermitian extension of $T$ is a hermitian restriction of $T^*$. The larger the domain of a hermitian operator the smaller the domain of its adjoint. The choice of the domain of $S$ has to be properly adjusted in order to get a self-adjoint extension of $T$; recall also that a self-adjoint operator is maximal, in the sense that it has no proper hermitian extensions.

**Definition 7.1.1.** Let $T$ be a hermitian operator. The *boundary form* of $T$ is the sesquilinear map $\Gamma = \Gamma_{T^*} : \mathrm{dom}\, T^* \times \mathrm{dom}\, T^* \to \mathbb{C}$ given by

$$\Gamma(\xi, \eta) := \langle T^*\xi, \eta\rangle - \langle \xi, T^*\eta\rangle\,, \qquad \xi, \eta \in \mathrm{dom}\, T^*.$$

$\Gamma(\xi)$ will also denote $\Gamma(\xi, \xi)$.

In case $T^*$ is known, $\Gamma$ can be used to find the closure of $T$, that is, $\overline{T}$. Since $\overline{T} = T^{**} \subset T^*$, by the definition of the adjoint operator $T^{**}$ one has that $\xi \in \mathrm{dom}\, \overline{T}$ iff there is $\eta \in \mathcal{H}$ with

$$\langle \xi, T^*\zeta\rangle = \langle \eta, \zeta\rangle\,, \qquad \forall \zeta \in \mathrm{dom}\, T^*,$$

and $\eta = \overline{T}\xi$. Since $\overline{T} \subset T^*$ one has $\eta = T^*\xi$ and so the above relation is equivalent to

$$0 = \Gamma(\xi, \zeta) = \langle T^*\xi, \zeta\rangle - \langle \xi, T^*\zeta\rangle , \qquad \forall \zeta \in \mathrm{dom}\ T^*,$$

which is a (anti)linear equation for $\xi \in \mathrm{dom}\ \overline{T}$.

*Exercise* 7.1.2. Use the above characterization of $\overline{T}$ to show that the closure of a hermitian operator is also hermitian.

**Proposition 7.1.3.** $\Gamma(\xi, \eta) = 0$, $\forall \xi, \eta \in \mathrm{dom}\ T^*$, *iff* $T^*$ *is self-adjoint, that is, iff* $T$ *is essentially self-adjoint.*

*Exercise* 7.1.4. Present a proof of Proposition 7.1.3. Hence, the boundary form $\Gamma$ quantifies the "lack of self-adjointness" of $T^*$.

**Proposition 7.1.5.** *If* $T$ *is hermitian then*

$$\mathrm{dom}\ \overline{T} = \{\xi \in \mathrm{dom}\ T^* : \Gamma(\xi, \eta_\pm) = 0, \forall \eta_\pm \in \mathrm{K}_\pm(T)\}.$$

*Proof.* Recall that if $\zeta \in \mathrm{dom}\ T^*$, then $\zeta = \eta + \eta_+ + \eta_-$, with $\eta \in \mathrm{dom}\ \overline{T}$, and $\eta_\pm \in \mathrm{K}_\pm(T)$ (the deficiency subspaces). Since $\Gamma(\xi, \eta) = 0$ for all $\xi \in \mathrm{dom}\ T^*, \eta \in \mathrm{dom}\ \overline{T}$, it follows that $\xi \in \mathrm{dom}\ \overline{T}$ iff for all $\zeta \in \mathrm{dom}\ T^*$

$$0 = \Gamma(\xi, \zeta) = \Gamma(\xi, \eta + \eta_+ + \eta_-) = \Gamma(\xi, \eta_+ + \eta_-).$$

The result follows. □

*Exercise* 7.1.6. Show that an operator $S$ so that $T \subset S \subset T^*$ is hermitian iff $\Gamma(\xi, \eta) = 0$ for all $\xi, \eta \in \mathrm{dom}\ S$.

Let $\zeta^1 = \eta^1 + \eta^1_+ + \eta^1_-$ and $\zeta^2 = \eta^2 + \eta^2_+ + \eta^2_-$, with $\eta^1, \eta^2 \in \mathrm{dom}\ \overline{T}$, $\eta^1_+, \eta^2_+ \in \mathrm{K}_+(T)$, $\eta^1_-, \eta^2_- \in \mathrm{K}_-(T)$, be general elements of $\mathrm{dom}\ T^*$; since $T^*\eta_\pm = \mp i\eta_\pm$, it follows by Theorem 2.2.11 that

$$\Gamma(\zeta^1, \zeta^2) = \Gamma(\eta^1_+ + \eta^1_-, \eta^2_+ + \eta^2_-) = 2i \left(\langle \eta^1_+, \eta^2_+\rangle - \langle \eta^1_-, \eta^2_-\rangle\right).$$

It is then clear that the nonvanishing of $\Gamma$ is related to the deficiency subspaces. Boundary forms can be used to determine self-adjoint extensions of $T$ by noting that such extensions are restrictions of $T^*$ on suitable domains $\mathcal{D}$ so that $\Gamma(\xi, \eta) = 0, \forall \xi, \eta \in \mathcal{D}$ (Lemma 7.1.7). Recall that each self-adjoint extension of $T$ is related to a unitary operator $\mathcal{U} : \mathrm{K}_-(T) \to \mathrm{K}_+(T)$ onto $\mathrm{K}_+(T)$; denote by $T_\mathcal{U}$ the corresponding self-adjoint extension, whose domain is $\mathrm{dom}\ T_\mathcal{U} = \{\eta = \zeta + \eta_- - \mathcal{U}\eta_- : \zeta \in \mathrm{dom}\ \overline{T}, \eta_- \in \mathrm{K}_-(T)\}$. Then, explicitly one has

**Lemma 7.1.7.** *The boundary form* $\Gamma_{T^*}$ *restricted to* $\mathrm{dom}\ T_\mathcal{U}$ *vanishes identically.*

*Proof.* For any two elements $\eta = \zeta_1 + \eta_- - \mathcal{U}\eta_-$ and $\xi = \zeta_2 + \xi_- - \mathcal{U}\xi_-$ in $\mathrm{dom}\ T_\mathcal{U}$ ($\zeta_1, \zeta_2 \in \mathrm{dom}\ \overline{T}$) one has

$$\Gamma(\xi, \eta) = 2i\,(\langle \mathcal{U}\xi_-, \mathcal{U}\eta_-\rangle - \langle \xi_-, \eta_-\rangle) = 0,$$

which vanishes since $\mathcal{U}$ is unitary. □

**Proposition 7.1.8.** *Assume that $T$ has self-adjoint extensions. Then each self-adjoint extension of $T$ is of the form*

$$\text{dom } T_{\mathcal{U}} = \{\xi \in \text{dom } T^* : \Gamma(\xi, \eta_- - \mathcal{U}\eta_-) = 0, \forall \eta_- \in \mathrm{K}_-(T)\},$$

$T_{\mathcal{U}}\xi = T^*\xi$, $\xi \in \text{dom } T_{\mathcal{U}}$ *($\mathcal{U}$ as above).*

*Proof.* If $T_{\mathcal{U}}$ is a self-adjoint extension of $T$, then $\text{dom } T_{\mathcal{U}} = \{\eta = \zeta + \eta_- - \mathcal{U}\eta_- : \zeta \in \text{dom } \overline{T}, \eta_- \in \mathrm{K}_-(T)\}$; since $\Gamma$ restricted to $\text{dom } T_{\mathcal{U}}$ vanishes, by Proposition 7.1.5 one has, for $\xi \in \text{dom } T_{\mathcal{U}}$,

$$0 = \Gamma(\xi, \zeta + \eta_- - \mathcal{U}\eta_-) = \Gamma(\xi, \eta_- - \mathcal{U}\eta_-), \qquad \forall \eta_- \in \mathrm{K}_-.$$

Hence, $\text{dom } T_{\mathcal{U}} \subset A := \{\xi \in \text{dom } T^* : \Gamma(\xi, \eta_- - \mathcal{U}\eta_-) = 0, \forall \eta_- \in \mathrm{K}_-(T)\}$.

Now, given $\mathcal{U}$, consider the linear equation for $\zeta + \xi_- + \xi_+ = \xi \in \text{dom } T^*$ (of course $\xi_\pm \in \mathrm{K}_\pm(T)$)

$$0 = \Gamma(\xi, \eta_- - \mathcal{U}\eta_-), \qquad \forall \eta_- \in \mathrm{K}_-(T).$$

By Lemma 7.1.7, any $\xi \in \text{dom } T_{\mathcal{U}}$ is a solution of this equation. Let $\xi \in \text{dom } T^*$ be a solution and write

$$\xi = \zeta + \xi_- - \mathcal{U}\xi_- + \xi_+ + \mathcal{U}\xi_-;$$

thus

$$\begin{aligned} 0 &= \Gamma(\xi, \eta_- - \mathcal{U}\eta_-) = \Gamma(\xi_- - \mathcal{U}\xi_- + \xi_+ + \mathcal{U}\xi_-, \eta_- - \mathcal{U}\eta_-) \\ &= 2i\left(\langle(\xi_+ + \mathcal{U}\xi_-) - \mathcal{U}\xi_-, \mathcal{U}\eta_-\rangle - \langle\xi_-, \eta_-\rangle\right) \\ &= 2i\left(\langle\xi_+ + \mathcal{U}\xi_-, -\mathcal{U}\eta_-\rangle + \langle\mathcal{U}\xi_-, \mathcal{U}\eta_-\rangle - \langle\xi_-, \eta_-\rangle\right) \\ &= 2i\,\langle\xi_+ + \mathcal{U}\xi_-, -\mathcal{U}\eta_-\rangle, \qquad \forall \eta_- \in K(T). \end{aligned}$$

Since $\text{rng } \mathcal{U} = \mathrm{K}_+$, it follows that $\xi_+ + \mathcal{U}\xi_- = 0$, or $\xi_+ = -\mathcal{U}\xi_-$; thus $\xi = \zeta + \xi_- - \mathcal{U}\xi_- \in \text{dom } T_{\mathcal{U}}$ so that $A \subset \text{dom } T_{\mathcal{U}}$. Therefore $\text{dom } T_{\mathcal{U}} = A$, and the proposition is proved. ☐

*Remark* 7.1.9. Note that the specification of the self-adjoint extensions $T_{\mathcal{U}}$ in Proposition 7.1.8 does not require the explicit knowledge of $\overline{T}$; sometimes this can be handy and an advantage over the specification presented in Section 2.5.

*Example* 7.1.10. As an illustration of the above ideas, the simple case of the momentum differential operator on a bounded interval $(a, b)$ of Example 2.3.14 will be discussed. Let

$$\text{dom } P = C_0^\infty(0,1) \sqsubseteq \mathcal{H} = \mathrm{L}^2[0,1],$$

$(P\psi)(x) = -i\psi'(x), \psi \in \text{dom } P$. On integrating by parts it is found that $P$ is hermitian. One has $\text{dom } P^* = \mathcal{H}^1[0,1]$ and $(P^*\psi)(x) = -i\psi'(x), \psi \in \text{dom } P^*$. In this case the boundary form is

$$\Gamma(\psi, \phi) = i\left(\overline{\psi(1)}\phi(1) - \overline{\psi(0)}\phi(0)\right), \qquad \psi, \phi \in \text{dom } P^*.$$

By choosing $\psi = \phi \in \mathcal{H}^1[0,1]$ with $\phi(0) = 0$ and $\phi(1) \neq 0$ one has $\Gamma(\phi) \neq 0$, and so $P^*$ is not self-adjoint; consequently $P$ is not essentially self-adjoint. Now $\psi$ is in the domain of the closure $\overline{P}$ iff

$$0 = \Gamma(\psi, \phi) = i\left(\overline{\psi(1)}\phi(1) - \overline{\psi(0)}\phi(0)\right), \qquad \forall \phi \in \mathcal{H}^1[0,1];$$

taking $\phi$ vanishing at only one end, it follows that $\psi(0) = 0 = \psi(1)$, that is, $\operatorname{dom} \overline{P} = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$. For the self-adjoint extensions Proposition 7.1.8 leads exactly to the characterization presented in Example 2.6.5, although now the specification of $\operatorname{dom} \overline{P}$ is not necessary.

### 7.1.1 Boundary Triples

A boundary triple is an abstraction of the notion of boundary values in function spaces; this idea goes back to Calkin in 1939 [Ca39] and Vishik in 1952 [Vi63].

**Definition 7.1.11.** Let $T$ be a hermitian operator in $\mathcal{H}$ with $n_-(T) = n_+(T)$. A *boundary triple* $(\mathbf{h}, \rho_1, \rho_2)$ for $T$ is composed of a Hilbert space $\mathbf{h}$ and two linear maps $\rho_1, \rho_2 : \operatorname{dom} T^* \to \mathbf{h}$ with dense ranges and so that

$$a\,\Gamma_{T^*}(\xi, \eta) = \langle \rho_1(\xi), \rho_1(\eta)\rangle - \langle \rho_2(\xi), \rho_2(\eta)\rangle, \ \forall \xi, \eta \in \operatorname{dom} T^*,$$

for some constant $0 \neq a \in \mathbb{C}$. Note that $\langle \cdot, \cdot \rangle$ is also denoting the inner product in $\mathbf{h}$.

In general, given a hermitian operator $T$ with equal deficiency indices, different boundary triples can be associated with it; since for $\zeta^1, \zeta^2 \in \operatorname{dom} T^*$ (by using the above notation)

$$\Gamma(\zeta^1, \zeta^2) = 2i\left(\langle \eta_+^1, \eta_+^2\rangle - \langle \eta_-^1, \eta_-^2\rangle\right),$$

only the deficiency subspaces effectively appear in the boundary form, consequently one may take either $\mathbf{h} = \mathrm{K}_-(T)$ or $\mathbf{h} = \mathrm{K}_+(T)$ (with $\rho$ properly chosen); in this case, say $\mathbf{h} = \mathrm{K}_-(T)$, by von Neumann theory it is known that self-adjoint extensions are in one-to-one relation with unitary operators $\mathcal{U} : \mathrm{K}_-(T) \to \mathrm{K}_+(T)$. However, it is convenient to allow a general $\mathbf{h}$ with $\dim \mathbf{h} = n_+(T)$ (recall that two Hilbert spaces are unitarily equivalent iff they have the same dimension), and Theorem 7.1.13 will adapt von Neumann theory to this situation.

Again, self-adjoint extensions of $T$ are restrictions of $T^*$ on suitable domains $\mathcal{D}$ so that $\Gamma(\xi, \eta) = 0, \forall \xi, \eta \in \mathcal{D}$, and given a boundary triple for $T$, such $\mathcal{D}$ are related to isometric maps $\hat{\mathcal{U}} : \mathbf{h} \to \mathbf{h}$ (which can be taken to be onto; extend it by continuity, if necessary) so that $\hat{\mathcal{U}}\rho_1(\xi) = \rho_2(\xi)$ and

$$\langle \rho_1(\xi), \rho_1(\eta)\rangle = \langle \rho_2(\xi), \rho_2(\eta)\rangle = \left\langle \hat{\mathcal{U}}\rho_1(\xi), \hat{\mathcal{U}}\rho_1(\eta)\right\rangle,$$

$\forall \xi, \eta \in \mathcal{D}$. Next the linearity of $\hat{\mathcal{U}}$ will be established.

**Lemma 7.1.12.** *Each* $\hat{\mathcal{U}}$ *above is a linear and unitary map.*

*Proof.* Note that rng $\hat{\mathcal{U}} = \mathbf{h}$ and it will suffice to show that this operator is invertible and linear. To simplify the notation, $\rho_1$ and $\rho_2$ will not appear in what follows.

If $\hat{\mathcal{U}}(\xi) = \hat{\mathcal{U}}(\eta)$, then

$$\begin{aligned}
0 &= \left\langle \hat{\mathcal{U}}(\xi) - \hat{\mathcal{U}}(\eta), \hat{\mathcal{U}}(\xi) - \hat{\mathcal{U}}(\eta) \right\rangle \\
&= \left\langle \hat{\mathcal{U}}(\xi), \hat{\mathcal{U}}(\xi) \right\rangle - \left\langle \hat{\mathcal{U}}(\xi), \hat{\mathcal{U}}(\eta) \right\rangle - \left\langle \hat{\mathcal{U}}(\eta), \hat{\mathcal{U}}(\xi) \right\rangle + \left\langle \hat{\mathcal{U}}(\eta), \hat{\mathcal{U}}(\eta) \right\rangle \\
&= \langle \xi, \xi \rangle - \langle \xi, \eta \rangle - \langle \eta, \xi \rangle + \langle \eta, \eta \rangle = \|\xi - \eta\|^2;
\end{aligned}$$

therefore $\xi = \eta$ and so $\hat{\mathcal{U}}$ is injective and $\hat{\mathcal{U}}^{-1} : \mathbf{h} \to \mathbf{h}$ exists.

If $\hat{\mathcal{U}}^{-1}(\xi_1) = \xi$ and $\hat{\mathcal{U}}^{-1}(\eta_1) = \eta$, since by hypothesis $\left\langle \hat{\mathcal{U}}(\xi), \hat{\mathcal{U}}(\eta) \right\rangle = \langle \xi, \eta \rangle$, $\forall \xi, \eta$, then $\langle \xi_1, \eta_1 \rangle = \left\langle \hat{\mathcal{U}}^{-1}(\xi_1), \hat{\mathcal{U}}^{-1}(\eta_1) \right\rangle$; since $\hat{\mathcal{U}}$ is bijective such a relation holds for every vector in the space. In this relation, if $\xi_1 = \hat{\mathcal{U}}(\xi_2)$, then $\left\langle \hat{\mathcal{U}}(\xi_2), \eta_1 \right\rangle = \left\langle \xi_2, \hat{\mathcal{U}}^{-1}(\eta_1) \right\rangle$, again for all vectors of $\mathbf{h}$.

Now, for all $\eta, \xi, \zeta \in \mathbf{h}$ and $a, b \in \mathbb{C}$, one has

$$\begin{aligned}
\left\langle \hat{\mathcal{U}}(a\xi + b\eta), \zeta \right\rangle &= \left\langle a\xi + b\eta, \hat{\mathcal{U}}^{-1}(\zeta) \right\rangle \\
&= \bar{a} \left\langle \xi, \hat{\mathcal{U}}^{-1}(\zeta) \right\rangle + \bar{b} \left\langle \eta, \hat{\mathcal{U}}^{-1}(\zeta) \right\rangle \\
&= \bar{a} \left\langle \hat{\mathcal{U}}(\xi), \zeta \right\rangle + \bar{b} \left\langle \hat{\mathcal{U}}(\eta), \zeta \right\rangle = \left\langle a\hat{\mathcal{U}}(\xi) + b\hat{\mathcal{U}}(\eta), \zeta \right\rangle,
\end{aligned}$$

showing that $\hat{\mathcal{U}}(a\xi + b\eta) = a\hat{\mathcal{U}}(\xi) + b\hat{\mathcal{U}}(\eta)$, that is, $\hat{\mathcal{U}}$ is linear. □

**Theorem 7.1.13.** *Let* $T$ *be a hermitian operator with equal deficiency indices. If* $(\mathbf{h}, \rho_1, \rho_2)$ *is a boundary triple for* $T$*, then the self-adjoint extensions* $T_{\hat{\mathcal{U}}}$ *of* $T$ *are precisely*

$$\text{dom } T_{\hat{\mathcal{U}}} = \left\{ \xi \in \text{dom } T^* : \rho_2(\xi) = \hat{\mathcal{U}} \rho_1(\xi) \right\}, \qquad T_{\hat{\mathcal{U}}}\xi = T^*\xi,$$

*for every unitary map* $\hat{\mathcal{U}} : \mathbf{h} \to \mathbf{h}$.

*Proof.* A necessary condition for the restriction of $T^*$ to a domain $\mathcal{D}$ be self-adjoint is that the corresponding boundary form vanishes identically on $\mathcal{D}$. Given the boundary triple, taking into account Lemma 7.1.12 and the discussion that precedes it, Lemma 7.1.7 and Proposition 7.1.8, such $\mathcal{D}$'s are necessarily obtained through unitary maps $\hat{\mathcal{U}} : \mathbf{h} \to \mathbf{h}$ and it is enough to check that actually each $T_{\hat{\mathcal{U}}}$ is self-adjoint.

Clearly $T_{\hat{\mathcal{U}}}$ is a hermitian extension of $T$. If $\eta \in \text{dom } T^*_{\hat{\mathcal{U}}}$ one has

$$\langle T^*_{\hat{\mathcal{U}}}\eta, \xi\rangle = \langle \eta, T_{\hat{\mathcal{U}}}\xi\rangle = \langle \eta, T^*_{\hat{\mathcal{U}}}\xi\rangle, \qquad \forall \xi \in \text{dom } T_{\hat{\mathcal{U}}}.$$

Then,

$$\begin{aligned} 0 = \Gamma_{T^*_{\hat{\mathcal{U}}}}(\eta,\xi) &= \langle T^*_{\hat{\mathcal{U}}}\eta, \xi\rangle - \langle \eta, T^*_{\hat{\mathcal{U}}}\xi\rangle \\ &= \langle \rho_1(\eta), \rho_1(\xi)\rangle - \langle \rho_2(\eta), \rho_2(\xi)\rangle \\ &= \langle \rho_1(\eta), \rho_1(\xi)\rangle - \langle \rho_2(\eta), \hat{\mathcal{U}}\rho_1(\xi)\rangle \\ &= \langle \rho_1(\eta), \rho_1(\xi)\rangle - \langle \hat{\mathcal{U}}^*\rho_2(\eta), \rho_1(\xi)\rangle \\ &= \langle \rho_1(\eta) - \hat{\mathcal{U}}^*\rho_2(\eta), \rho_1(\xi)\rangle, \qquad \forall \xi \in \text{dom } T_{\hat{\mathcal{U}}}. \end{aligned}$$

Since $\rho_1$ has dense range in $\mathbf{h}$, it follows that $\rho_1(\eta) - \hat{\mathcal{U}}^*\rho_2(\eta) = 0$, that is, $\rho_2(\eta) = \hat{\mathcal{U}}\rho_1(\eta)$ and $\eta \in \text{dom } T_{\hat{\mathcal{U}}}$. Therefore, $T_{\hat{\mathcal{U}}}$ is self-adjoint. □

Often a boundary triple for differential operators gives self-adjoint extensions in terms of boundary conditions, and different choices of the triple correspond to different parametrizations of such extensions. In applications sometimes it is convenient to distinguish the spaces $\rho_1(\mathbf{h})$ from $\rho_2(\mathbf{h})$ by different symbols.

*Remark* 7.1.14. The definition of boundary triple presented here is slightly different from the current definition in the literature; maybe the term *modified boundary triple* should be used. For the usual approach and related results and references in case of differential operators see [GorG91] and [BrGP08].

## 7.2 Schrödinger Operators on Intervals

Important Schrödinger operators are self-adjoint extensions of the minimal operator

$$H = -\frac{d^2}{dx^2} + V(x), \qquad \text{dom } H = C_0^\infty(a,b) \sqsubseteq \mathrm{L}^2(a,b),$$

with $-\infty \le a < b \le +\infty$; the weakest request on the (real-valued) potential is $V \in \mathrm{L}^2_{\text{loc}}(a,b)$, and this will be henceforth supposed in this chapter.

Note that $\mathrm{L}^2(a,b) = \mathrm{L}^2[a,b]$ since the set of end points $\{a,b\}$ has zero Lebesgue measure. However, in case of bounded intervals one has $C_0^\infty(a,b) \neq C_0^\infty[a,b]$ and for absolutely continuous functions $\mathrm{AC}(a,b) \neq \mathrm{AC}[a,b]$ (recall that $\mathrm{AC}(a,b)$ denotes the set of absolutely continuous functions in every bounded and closed interval $[c,d] \subset (a,b)$). By Proposition 2.2.16, $H$ has equal deficiency indices and so self-adjoint extensions do exist. In this and the next sections some results related to this matter will be addressed, as well as some ways of getting self-adjoint extensions of $H$, mainly illustrated by means of boundary forms. In this section $H$ always refers to this minimal differential operator.

Again note the open interval $(a, b)$ and in general $V \in \mathrm{L}^2_{\mathrm{loc}}$ is allowed to "drastically diverge" at the end points. For $V \in \mathrm{L}^2_{\mathrm{loc}}(a, b)$, Proposition 2.3.20 ensures that dom $H^*$ equals

$$\left\{\psi \in \mathrm{L}^2(a,b) : \psi, \psi' \in \mathrm{AC}(a,b), (-\psi'' + V\psi) \in \mathrm{L}^2(a,b)\right\},$$

so that if $\psi \in$ dom $H^*$ then $\psi, \psi'$ are absolutely continuous functions in $(a, b)$, and in case the potential $V$ has a discontinuity at a point $c \in (a, b)$, then $\psi$ and $\psi'$ must be continuous at $c$ for any $\psi$ in the domain of a self-adjoint extension of $H$. Such continuity conditions at $c$ are habitually imposed on wave functions (i.e., $\psi$) in quantum mechanics textbooks, and here the justification is seen to be related to regularity properties of elements of dom $H^*$.

**Lemma 7.2.1.** *The boundary form of the above minimal operator $H$ is*

$$\Gamma(\psi, \varphi) = W_b[\psi, \varphi] - W_a[\psi, \varphi], \qquad \psi, \varphi \in \mathrm{dom}\ H^*,$$

*where $W_x[\psi, \varphi] = \overline{\psi(x)}\varphi'(x) - \overline{\psi'(x)}\varphi(x)$ is the wronskian of $\psi, \varphi$ at $x \in (a, b)$, and $W_a[\psi, \varphi] := \lim_{x \to a^+} W_x[\psi, \varphi]$, $W_b[\psi, \varphi] := \lim_{x \to b^-} W_x[\psi, \varphi]$.*

*Proof.* Let $[c, d] \subset (a, b)$ and $\psi, \varphi \in$ dom $H^*$. In view of $V \in \mathrm{L}^2_{\mathrm{loc}}(a, b)$, on integrating by parts one gets that $\Gamma(\psi, \phi)$ is reduced to

$$\int_c^d \left(\overline{(H^*\psi)(x)}\varphi(x) - \overline{\psi(x)}(H^*\varphi)(x)\right) dx = W_d[\psi, \varphi] - W_c[\psi, \varphi];$$

since the integral over the whole interval $[a, b]$ is finite, the limits defining $W_a[\psi, \varphi]$ and $W_b[\psi, \varphi]$ exist (modify the functions so that they vanish in a neighborhood of $a$; then $W_b[\psi, \varphi]$ exists; similarly for the other end) and $\Gamma(\psi, \varphi) = W_b[\psi, \varphi] - W_a[\psi, \varphi]$. □

*Exercise* 7.2.2. Let $H$ be the above minimal operator and $u \in \mathrm{L}^1_{\mathrm{loc}}(a, b)$. If $\psi, \varphi$ are solutions of $H^*\psi = u$, show that the wronskian $W_x[\overline{\psi}, \varphi] = \gamma$ is constant. Furthermore, if $\{\overline{\psi}, \varphi\}$ is a linearly independent set, show that such a constant $\gamma \neq 0$, and given $c \in (a, b)$,

$$\phi(x) := \frac{1}{\gamma} \int_c^x \left[\psi(x)\varphi(t) - \varphi(x)\psi(t)\right] u(t)\, dt$$

is the unique solution of $H^*\psi = u$ with initial conditions $\phi(c) = 0$ and $\phi'(c) = 0$.

### 7.2.1 Regular and Singular End Points

**Definition 7.2.3.** The end point $a$ is *regular* for the differential operator $H = -d^2/dx^2 + V$ if $-\infty < a$ and for some $c \in (a, b)$ (and so for all such $c$) one has $\int_a^c |V(x)|\, dx := \lim_{d \to a^+} \int_d^c |V(x)|\, dx < \infty$; $b$ is regular for $H$ if $b < \infty$ and $\int_c^b |V(x)|\, dx := \lim_{d \to b^-} \int_c^d |V(x)|\, dx < \infty$. If an end point is not regular it is called *singular*.

From the theory of differential equations [Na69] it is known that the space of solutions of the K$_{\mp}$-*equation*

$$H^*\psi = -\psi'' + V\psi = \pm i\psi, \qquad \psi \in \text{dom } H^*,$$

is two-dimensional and if $a$ is a regular point for $H$ then any solution $\psi$ has finite limits $\psi(a) := \psi(a^+) = \lim_{x\to a^+}\psi(x)$ and $\psi'(a) := \psi'(a^+) = \lim_{x\to a^+}\psi'(x)$; if $a$ is singular then such limits can be divergent.

Recall also that if $V$ is a continuous function (even complex-valued) on $(a,b)$, then any solution of

$$-\psi'' + (V - z)\psi = 0, \qquad z \in \mathbb{C},$$

is a twice continuously differentiable function in $(a,b)$, and in case $V \in C^\infty(a,b)$ then $\psi \in C^\infty(a,b)$.

**Proposition 7.2.4.** *Let $H$ be the above minimal differential operator.*

i) *The closure of $H$ is given by*

$$\text{dom } \overline{H} = \{\psi \in \text{dom } H^* : W_b[\psi,\varphi] = 0, W_a[\psi,\varphi] = 0, \forall\varphi \in \text{dom } H^*\},$$
$$\overline{H}\psi = H^*\psi, \qquad \forall\psi \in \text{dom } \overline{H}.$$

ii) *Let $\psi \in \text{dom } H^*$. In case $a$ is a regular end point, then the condition $W_a[\psi,\varphi] = 0$, $\forall\varphi \in \text{dom } H^*$, means $\psi(a) = 0 = \psi'(a)$ (similarly for $b$).*

*Proof.* i) Combine Proposition 7.1.5 and Lemma 7.2.1 to get

$$\text{dom } \overline{H} = \{\psi \in \text{dom } H^* : W_b[\psi,\varphi] - W_a[\psi,\varphi] = 0, \forall\varphi \in \text{dom } H^*\}.$$

Since the behavior of functions in dom $H^*$ near $a$ is independent of their values near $b$, it follows that the statement $W_b[\psi,\varphi] - W_a[\psi,\varphi] = 0, \forall\varphi \in \text{dom } H^*$, is equivalent to $W_b[\psi,\varphi] = 0 = W_a[\psi,\varphi], \forall\varphi \in \text{dom } H^*$ (e.g., given $\varphi$, pick $u \in$ dom $H^*$ that coincides with $\varphi$ in a neighborhood of $a$ and is zero in a neighborhood of $b$; then $W_a[\psi,\varphi] = W_a[\psi,u] = W_b[\psi,u] = 0$).

ii) If $a$ is a regular point, then $\varphi(a), \varphi'(a)$ are well defined (i.e., they have finite limits) for all $\varphi \in \text{dom } H^*$; hence $0 = W_a[\psi,\varphi] = \overline{\psi(a)}\varphi'(a) - \overline{\psi'(a)}\varphi(a)$, $\forall\varphi \in \text{dom } H^*$, implies $\psi(a) = 0 = \psi'(a)$, since $\varphi(a), \varphi'(a)$ can take arbitrary values. □

**Corollary 7.2.5.** *If both end points $a, b$ are regular, then*

$$\text{dom } \overline{H} = \{\psi \in \text{dom } H^* : \psi(b) = \psi'(b) = 0 = \psi(a) = \psi'(a)\}.$$

**Corollary 7.2.6.** *If $H$ has a regular end point, then its closure $\overline{H}$ has no eigenvalues.*

*Proof.* Say $a$ is a regular end point. Then the solution of $\overline{H}\psi = \lambda\psi$, $\psi \in \text{dom } \overline{H}$, $\lambda \in \mathbb{C}$, must satisfy $\psi(a) = 0 = \psi'(a)$, and so, by uniqueness, $\psi$ is the null solution. □

**Definition 7.2.7.** A measurable function $u : (a,b) \to \mathbb{C}$ is in $\mathrm{L}^2$ *near the end point* $a$ if there exists $c \in (a,b)$ so that $u \in \mathrm{L}^2(a,c)$ (in fact the restriction $u|_{(a,c)} \in \mathrm{L}^2(a,c)$); similarly for $u$ that is $\mathrm{L}^2$ near $b$.

*Remark* 7.2.8. Note that if $\psi$ is a solution of the $\mathrm{K}_-$-equation for $H$, then $\overline{\psi}$ is a solution of the corresponding $\mathrm{K}_+$-equation. So for each solution $\mathrm{L}^2$ near $a$ of the $\mathrm{K}_-$-equation corresponds a solution $\mathrm{L}^2$ near $a$ of the $\mathrm{K}_+$-equation and vice versa. Similarly for the end point $b$.

**Theorem 7.2.9.** *Let $H$ be the minimal operator introduced on page* 174.

i) *The deficiency indices of the above minimal operator $H$ are finite and bounded by $0 \le n_-(H) = n_+(H) \le 2$.*
ii) *If both end points $a, b$ are regular, then $n_-(H) = n_+(H) = 2$.*

*Proof.* i) By Proposition 2.2.16, $n_-(H)=n_+(H)$. From the above discussion on solutions of linear differential equations of second order one has, say, $0 \le n_-(H) \le 2$.

ii) If $u$ is a solution of

$$H^*\psi = -\psi'' + V\psi = -i\psi, \qquad \psi \in \mathrm{dom}\ H^*,$$

then $u, u'$ are absolutely continuous in $(a,b)$ and so for any $[c,d] \subset (a,b)$ one has $\int_c^d |u(x)|^2\, dx < \infty$. Since the limits $u(a^+), u(b^-)$ exist and $a, b$ are finite, one gets $\int_a^b |u(x)|^2\, dx < \infty$, consequently all elements of $\mathrm{K}_+(H)$ are in $\mathrm{L}^2[a,b]$. Hence $n_+(H) = 2$. By item i), $n_-(H) = 2$. □

**Lemma 7.2.10.** *Let $H$ be the minimal operator introduced on page* 174. *For each end point, at least one* (*nonzero*) *solution of*

$$H^*\psi = -\psi'' + V\psi = \pm i\psi, \qquad \psi \in \mathrm{dom}\ H^*,$$

*is* $\mathrm{L}^2$ *near it.*

*Proof.* Let $a, b$ be the end points and $a < a' < b' < b$; it is enough to consider $-i$ on the right-hand side of the above equation, since the arguments are the same for the other possibility.

For the hermitian operator $\mathrm{dom}\ S = \{\psi, \psi' \in \mathrm{AC}[a',b'] \subset \mathrm{L}^2[a',b'] : \psi(a') = \psi'(a') = 0 = \psi(b') = \psi'(b')\}$,

$$S\psi = -\psi'' + V\psi,$$

$a', b'$ are regular end points and, by Theorem 7.2.9, $n_-(S) = 2 = n_+(S)$. Thus, $\overline{\mathrm{rng}\ (S + i\mathbf{1})} = \mathrm{K}_-(S)^\perp \ne \{0\}$, and since $C_0^\infty(a',b') \sqsubseteq \mathrm{L}^2[a',b']$, there exists $\phi \in C_0^\infty(a',b')$ with $\phi \notin \mathrm{rng}\ (S + i\mathbf{1})$. Let $\hat{H}$ be a self-adjoint extension of $H$ and $\psi \in \mathrm{dom}\ \hat{H} \subset \mathrm{dom}\ H^*$ with $(\hat{H} + i\mathbf{1})\psi = \phi$ (recall that $\mathrm{rng}\ (\hat{H} + i\mathbf{1}) = \mathcal{H}$ by Proposition 2.2.4); note that the support of $\psi$ does not lie in $(a',b')$, for otherwise $\psi$ would belong to $\mathrm{dom}\ S$ and $(S + i\mathbf{1})\psi = \phi$, so that a contradiction would arise.

Now suppose that $\psi$ does not vanish identically on $(a, a')$ (similarly if it does not vanish identically on $(b', b)$). Then the restriction $u := \psi|_{(a,a')}$ is a solution of the above equation in the statement of the lemma (recall that $\hat{H} \subset H^*$) and it is $\mathrm{L}^2$ near $a$. The construction of the solution $\mathrm{L}^2$ near $b$ is as follows.

Consider the operator dom $Q = \{\varphi \in \mathrm{dom}\ \hat{H} : \varphi(x) = 0, \forall x \in [b', b)\}$ (under restriction, this set is dense in $\mathrm{L}^2(a, a')$), $Q := \hat{H}|_{\mathrm{dom}\ Q}$; in view of $u \in \mathrm{dom}\ Q$ and

$$Qu = -u'' + Vu = -iu,$$

it is found that $\bar{u} \in \mathrm{dom}\ Q^*$ (the complex conjugate of $u$ above) and

$$(Q^* - i\mathbf{1})\bar{u} = 0;$$

it then follows that rng $(Q + i\mathbf{1})$ is not dense and, as above, there exists $\phi \in C_0^\infty(a, a')$ with $\phi \notin \mathrm{rng}\ (Q + i\mathbf{1})$. The self-adjointness of $\hat{H}$ implies that rng $(\hat{H} + i\mathbf{1}) = \mathrm{L}^2(a, b)$, and so there is $v \in \mathrm{dom}\ \hat{H}$ with $(\hat{H} + i\mathbf{1})v = \phi$. Finally, $v$ does not vanish identically on $[b', b)$ since $\phi \notin \mathrm{rng}\ (Q + i\mathbf{1})$, and so a (nonzero) $\mathrm{L}^2$ near $b$ solution of the equation in the statement of the lemma was found. This completes the proof. □

**Corollary 7.2.11.** *If $n_-(H) = n_+(H) = 0$, that is, $H$ is essentially self-adjoint, then both ends $a, b$ are singular.*

*Proof.* If one end is regular then all solutions of the corresponding $\mathrm{K}_\mp$-equation are $\mathrm{L}^2$ near it and, by Lemma 7.2.10, there is at least one solution of the above equation that is $\mathrm{L}^2$ near the other end point, so at least one solution belongs to $\mathrm{L}^2(a, b)$ and $n_+(H) \geq 1$. Both ends being singular is the only remaining possibility if $n_- = n_+ = 0$. □

### 7.2.2 Limit Point, Limit Circle

Corollary 7.2.11 shows that a necessary condition for $H$ to be essentially self-adjoint is that both ends $a, b$ are singular. This is related to interesting results by Weyl (around 1910) and further developed by Levinson, Friedrichs and many others. For details justifying the terms in the next definition – although not immediate, they are quite interesting – consult [CoL55] or [Pea88].

**Definition 7.2.12.** The minimal differential operator $H$ is in the *limit point* (resp. *limit circle*) at one end point if the vector space of solutions of the $\mathrm{K}_\pm$-equation that are $\mathrm{L}^2$ near this end point is unidimensional (resp. two-dimensional).

**Theorem 7.2.13 (Weyl).** *The operator $H$ is essentially self-adjoint iff it is in the limit point at both ends $a$ and $b$.*

*Proof.* By Corollary 7.2.11 and the proof of Lemma 7.2.10, if $H$ is essentially self-adjoint, then both ends are limit point and the unique nonzero solution $\varphi$ of the $\mathrm{K}_+$-equation that is $\mathrm{L}^2$ near $a$ and the unique nonzero solution $\psi$ that is $\mathrm{L}^2$ near $b$ compose a linearly independent set, so that no solution belongs to $\mathrm{L}^2(a, b)$.

The task now is to show that if $H$ is limit point at both end points, then $n_- = n_+ = 0$, which is equivalent to $H^*$ being self-adjoint.

By Lemma 7.2.1,

$$\Gamma_{H^*}(\psi, \varphi) = W_b[\psi, \varphi] - W_a[\psi, \varphi], \qquad \forall \psi, \varphi \in \mathrm{dom}\ H^*;$$

also $H^*$ is self-adjoint iff the boundary form $\Gamma_{H^*}$ vanishes identically. Let $c \in (a, b)$ and $A, B$ be operators with the same action as $H$ but domains $\mathrm{dom}\ B = C_0^\infty(a, c)$ and $\mathrm{dom}\ A = \{\varphi \in C^\infty(a, c) : \varphi(c) = 0, \exists \varepsilon > 0, \varphi(x) = 0, \forall x \in (a, a + \varepsilon)\}$. Since $B \subset A$ one has $\overline{B} \subset \overline{A}$.

**Claim.** $\overline{A}$ is self-adjoint.

In fact, by hypothesis the solutions of $-\varphi'' + V\varphi = \pm i\varphi$ that are $\mathrm{L}^2$ near $a$ constitute a one-dimensional subspace, and since $c$ is a regular end point, all solutions are $\mathrm{L}^2$ near $c$; hence $n_-(B) = 1 = n_+(B)$. By noting that $\overline{A}$ is a proper hermitian extension of $\overline{B}$ (there are functions $\varphi$ in $\mathrm{dom}\ \overline{A}$ with $\varphi'(c) \neq 0$, but not in $\mathrm{dom}\ \overline{B}$; see Proposition 7.2.4), it follows that $n_\pm(\overline{A}) < n_\pm(\overline{B})$ (because $n_\pm(\overline{B}) < \infty$) and the unique possibility is then $n_-(A) = 0 = n_+(A)$, and so $\overline{A}$ is self-adjoint.

Let $\psi, \varphi \in \mathrm{dom}\ H^*$. Pick $\psi_c, \varphi_c \in C_0^\infty(a, b)$ so that both functions $\psi_2 := \psi + \psi_c$, $\varphi_2 := \varphi + \varphi_c$ vanish at $c$. Then, $\psi_2, \varphi_2 \in \mathrm{dom}\ \overline{A}$ and in view of $W_c[\psi_2, \varphi_2] = 0$ one finds

$$\begin{aligned} W_a[\psi, \varphi] &= W_a[\psi_2 - \psi_c, \varphi_2 - \varphi_c] = W_a[\psi_2, \varphi_2] \\ &= W_a[\psi_2, \varphi_2] - W_c[\psi_2, \varphi_2] = -\Gamma_{\overline{A}}(\psi_2, \varphi_2) = 0, \end{aligned}$$

since $\overline{A}$ is self-adjoint (see Lemma 7.1.7). Similar arguments show that $W_b[\psi, \varphi] = 0$, so that $\Gamma_{H^*}$ vanishes identically on $\mathrm{dom}\ H^*$ and $H^*$ is self-adjoint. Thereby the proof is complete. □

*Exercise* 7.2.14. Show that $H$ has deficiency indices $n_+ = n_- = 1$ iff it is limit circle at one end and limit point at the other.

*Example* 7.2.15. If $V$ is a real polynomial and $H\psi = -\psi'' + V\psi$, $\mathrm{dom}\ H = C_0^\infty(a, b)$ and $(a, b)$ a bounded interval, then both ends are regular and so $n_+ = n_- = 2$. Note that such a conclusion holds also for any continuous potential in $[a, b]$, including the free particle in the interval, that is, $V = 0$ (cf. Example 2.6.8).

*Example* 7.2.16. Let $V(x) = \kappa \ln(\gamma x)$, $\kappa \neq 0, \gamma > 0$, and $\mathrm{dom}\ H = C_0^\infty(0, 1)$. Since $V$ is regular at both end points, it follows that $n_- = n_+ = 2$.

*Exercise* 7.2.17. Show that the deficiency indices of $H$ in $(0, 1)$ with potential $V(x) = \kappa(\ln x)^2$ are equal to 2. Generalize for $V(x) = \kappa(\ln x)^m$, for any $\kappa \in \mathbb{R}, m \in \mathbb{N}$.

*Example* 7.2.18. Let $V(x) = \kappa/x^2$, $\kappa \neq 0$, and $H$ with $\mathrm{dom}\ H = C_0^\infty(0, 1)$. By Proposition 2.3.20, $\mathrm{dom}\ H^* = \{\psi \in \mathrm{L}^2(0, 1) : \psi, \psi' \in \mathrm{AC}(0, 1), (-\psi'' + \kappa/x^2\psi) \in$

$L^2(0,1)\}$. The end point 1 is regular, while 0 is not; so $H$ is limit circle at 1. For the end point 0 one needs to determine the solutions of the $K_\mp$-equation

$$H^*\psi = -\psi'' + \frac{\kappa}{x^2}\psi = \pm i\psi;$$

if one searches for solutions in the form $\psi(x) = x^a$, it follows that

$$-a(a-1)x^a + \kappa x^a \mp i x^{a+2} = 0,$$

so that, whether for $x \to 0$ the term $x^{a+2}$ could be ignored in comparison with the other terms, then one has approximately $-a(a-1) + \kappa = 0$, whose solutions are $a_\pm = 1/2(1 \pm \sqrt{1+4\kappa})$. If $-1/4 < \kappa < 3/4$ both solutions are independent and $L^2$ near 0 (so limit circle), whereas for $\kappa \geq 3/4$ only one of them is in $L^2$ near 0 (so limit point). Hence, $n_- = n_+ = 1$ if $\kappa \geq 3/4$ and $n_- = n_+ = 2$ if $-1/4 < \kappa < 3/4$.

Now a justification of the above procedure for $x \to 0$. If $\psi \in \operatorname{dom} H^*$, then

$$u = H^*\psi = -\psi'' + \frac{\kappa}{x^2}\psi \ \in L^2(0,1);$$

this may be thought of as a nonhomogeneous second-order linear differential equation for $\psi$. Note that the independent solutions of the homogeneous equation are exactly the above $\psi_+(x) = x^{a_+}$ and $\psi_-(x) = x^{a_-}$. By the well-known variation of parameters technique one obtains the general solution, that is,

$$\begin{aligned}\psi(x) =& \, b_+\psi_+(x) + b_-\psi_-(x)\\ &+ \left[\psi_+(x)\int_0^x \frac{\psi_-(t)u(t)}{W_t[\overline{\psi_+},\psi_-]}dt - \psi_-(x)\int_0^x \frac{\psi_+(t)u(t)}{W_t[\overline{\psi_+},\psi_-]}dt\right],\end{aligned}$$

for some constants $b_\pm$. A direct calculation gives $W_t[\overline{\psi_+},\psi_-] = -\gamma$, $\forall t$, with $\gamma = \sqrt{1+4\kappa}$. Write $\|u\|_{2,x} = \left(\int_0^x |u(t)|^2 dt\right)^{1/2}$ and note that $\|u\|_{2,x} \to 0$ as $x \to 0^+$. The absolute value of the term in square brackets is estimated from above by using Cauchy-Schwarz,

$$\begin{aligned}&\frac{\|u\|_{2,x}}{\gamma} \times \left(|\psi_+(x)|\left(\int_0^x |\psi_-(t)|^2\right)^{1/2} + |\psi_-(x)|\left(\int_0^x |\psi_+(t)|^2\right)^{1/2}\right)\\ &\qquad \leq \frac{4}{|4-\gamma^2|}\frac{\|u\|_{2,x}}{\gamma}x^{3/2}, \qquad -\frac{1}{4} < \kappa < \frac{3}{4}.\end{aligned}$$

The case $\kappa = 3/4$ is left as an exercise. Since such a term is in $L^2$ near 0, the final analysis of $\psi$ near 0 is left to the solutions of the homogeneous equation $\psi_+(x) = x^{a_+}$ and $\psi_-(x) = x^{a_-}$, which is exactly the analysis performed above.

*Exercise* 7.2.19. Discuss the case $\kappa = 3/4$ in Example 7.2.18 (see also Exercise 7.2.23).

*Exercise* 7.2.20. For $\psi \in \operatorname{dom} H^*$ in Example 7.2.18, find the behavior of $\psi'(x)$ for $x \to 0^+$.

*Example* 7.2.21. This is the potential of Example 7.2.18, but on the half-line. Let $V(x) = \kappa/x^2$, $\kappa \neq 0$, and $H$ with dom $H = C_0^\infty(0,\infty)$. The same conclusions about the end point 0 as in Example 7.2.18 are obtained. For the other end point consider the $K_-$-equation

$$-x^2\psi'' + \kappa\psi = ix^2\psi;$$

for $x \to \infty$ its solutions are governed by the equation $-\psi'' = i\psi$ whose solutions are $u_\pm(x) = e^{\pm(1\pm i)x/\sqrt{2}}$; since only one of them is in $L^2$ near $\infty$ (analogously to the $K_+$-equation), one concludes that $H$ is in the limit point at $\infty$ for all $\kappa \neq 0$. Therefore, if $\kappa \geq 3/4$ the operator $H$ is essentially self-adjoint, whereas $n_- = n_+ = 1$ if $-1/4 < \kappa < 3/4$.

For the justification of the above argument in case $x \to \infty$, apply Proposition 7.5.3 and Exercise 7.5.6.

*Exercise* 7.2.22. Check that

$$u_1(x) = \sqrt{x}\,\cos(t\ln x)/\sqrt{t}, \qquad u_2(x) = \sqrt{x}\,\sin(t\ln x)/\sqrt{t},$$

with $t = \sqrt{-\kappa - 1/4}$, $\kappa < -1/4$, are solutions of $-\psi'' + \frac{\kappa}{x^2}\psi = 0$.

*Exercise* 7.2.23. Show that the deficiency indices of dom $H = C_0^\infty(0,\infty)$, $H\psi = -\psi'' - \psi/(4x^2)$ are $n_- = 1 = n_+$. Note that $\psi_+(x) = \sqrt{x}$ and $\psi_-(x) = \sqrt{x}\ln x$ are solutions of $H^*\psi = 0$.

## 7.3 Regular Examples

In this section boundary triples will be used to get explicitly self-adjoint extensions of $H$ with regular end points. The ideas can be adapted to other situations.

*Example* 7.3.1. [Free particle on a half-line] The initial energy operator is $H\psi = -\psi''$, dom $H = C_0^\infty(0,\infty)$; by Example 2.3.19, $n_- = n_+ = 1$. Also dom $H^* = \mathcal{H}^2[0,\infty)$ and the boundary form, for $\psi, \varphi \in$ dom $H^*$, is readily seem to be

$$\Gamma(\psi,\varphi) = W_\infty[\psi,\varphi] - W_0[\psi,\varphi] = \overline{\psi'(0)}\varphi(0) - \overline{\psi(0)}\varphi'(0),$$

since the elements of dom $H^*$ vanish at infinity. Now define the vector spaces $X := \{\Psi = \psi(0) - i\psi'(0) : \psi \in \text{dom } H^*\}$ and the map $Y = \rho(X) := \{\rho(\Psi) = \psi(0) + i\psi'(0) : \Psi \in X\}$, and observe that

$$\langle\Psi,\Phi\rangle - \langle\rho(\Psi),\rho(\Phi)\rangle = 2i\Gamma(\psi,\varphi)$$

(of course $\Phi = \varphi(0) - i\varphi'(0)$), so that a boundary triple was found (with respect to Definition 7.1.11, think of $X = \rho_1(\text{dom } H^*)$ and $Y = \rho_2(\text{dom } H^*) = \rho(X)$).

Now, according to Theorem 7.1.13, a domain $\mathcal{D}$ so that $H^*|_\mathcal{D}$ is self-adjoint is characterized by unitary maps between $X$ and $Y$. Since $X$ and $Y$ are unidimensional, such unitary maps are multiplication by $e^{i\theta}$ for some $0 \leq \theta < 2\pi$. Therefore, the domain of self-adjoint extensions of $H$ are so that $\Psi = e^{i\theta}\rho(\Psi)$ for all $\Psi \in X$. Writing out such a relation

$$\psi(0) - i\psi'(0) = e^{i\theta}\left(\psi(0) + i\psi'(0)\right),$$

and so $(1 - e^{i\theta})\psi(0) = i(1 + e^{i\theta})\psi'(0)$; if $\theta \neq 0$ one has

$$\psi(0) = \lambda\psi'(0), \qquad \lambda = i\frac{(1 + e^{i\theta})}{(1 - e^{i\theta})} \in \mathbb{R}.$$

Therefore the self-adjoint extensions $H_\lambda$ of $H$ are characterized by the following boundary conditions

$$\text{dom } H_\lambda = \{\psi \in \mathcal{H}^2[0,\infty) : \psi(0) = \lambda\psi'(0)\}, \qquad H_\lambda\psi = -\psi'',$$

for each $\lambda \in \mathbb{R} \cup \{\infty\}$. The value $\lambda = \infty$ is for including $\theta = 0$, which corresponds to Neumann boundary condition $\psi'(0) = 0$. A Dirichlet boundary condition occurs for $\lambda = 0$. Exercises 7.3.2 and 11.6.11 discuss the spectra of such operators.

*Exercise* 7.3.2. Show that the self-adjoint operators $H_\lambda$ in Example 7.3.1 have an eigenvalue $E$ iff $\lambda < 0$ and $E = -1/\lambda^2$, whose eigenfunction is $\psi_E(x) = e^{x/\lambda}$. The existence of a negative value in the spectrum can be considered rather unexpected, since the actions of $H_\lambda$ indirectly suggest they are positive operators; the question is the boundary condition choice. Maybe, someone could discard such possibilities on the basis of physical arguments.

*Exercise* 7.3.3. Check that if in Example 7.2.21 one takes $\kappa = 0$, then Example 7.3.1 is recovered.

*Example* 7.3.4. [Free particle on an interval] The initial energy operator is $H\psi = -\psi''$, dom $H = C_0^\infty(0,1)$; by Example 7.2.15, $n_- = n_+ = 2$. Also dom $H^* = \mathcal{H}^2[0,1]$ and the boundary form is, for $\psi, \varphi \in \text{dom } H^*$,

$$\begin{aligned}\Gamma(\psi,\varphi) &= W_1[\psi,\varphi] - W_0[\psi,\varphi] \\ &= \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) - \overline{\psi(0)}\varphi'(0) + \overline{\psi'(0)}\varphi(0).\end{aligned}$$

Based on Example 7.3.1, define the two-dimensional vector spaces of elements

$$\Psi = \begin{pmatrix}\psi'(0) - i\psi(0) \\ \psi'(1) + i\psi(1)\end{pmatrix}, \qquad \rho(\Psi) = \begin{pmatrix}\psi'(0) + i\psi(0) \\ \psi'(1) - i\psi(1)\end{pmatrix},$$

for $\psi \in \text{dom } H^*$. A direct evaluation of inner products leads to

$$\langle\Psi,\Phi\rangle - \langle\rho(\Psi),\rho(\Phi)\rangle = -2i\Gamma(\psi,\varphi),$$

and a boundary triple was found.

By Theorem 7.1.13, a domain $\mathcal{D}$ so that $H^*|_{\mathcal{D}}$ is self-adjoint is characterized by a unitary $2\times 2$ matrix $\hat{U}$ so that $\Psi = \hat{U}\rho(\Psi)$ for all $\Psi$; recall that the general form of such matrices is

$$\hat{U} = e^{i\theta}\begin{pmatrix} a & -\bar{b} \\ b & \bar{a}\end{pmatrix}, \qquad \theta \in [0,2\pi),\ a,b \in \mathbb{C}, |a|^2 + |b|^2 = 1.$$

Writing out such a relation one obtains the boundary conditions

$$\left(\mathbf{1}-\hat{U}\right)\begin{pmatrix}\psi'(0)\\ \psi'(1)\end{pmatrix} = -i\left(\mathbf{1}+\hat{U}\right)\begin{pmatrix}-\psi(0)\\ \psi(1)\end{pmatrix}$$

and the domain of the corresponding self-adjoint extension $H_{\hat{U}}$ of $H$ is composed of the elements $\psi \in \mathcal{H}^2[0,1]$ so that the above boundary conditions are satisfied; also $H_{\hat{U}}\psi = -\psi''$. Some particular choices of $\hat{U}$ appear in exercises.

In case $(\mathbf{1}+\hat{U})$ is invertible (similarly if $(\mathbf{1}-\hat{U})$ is invertible) one can write the above boundary conditions as

$$A\begin{pmatrix}\psi'(0)\\ \psi'(1)\end{pmatrix} = \begin{pmatrix}-\psi(0)\\ \psi(1)\end{pmatrix}, \qquad A = i\left(\mathbf{1}+\hat{U}\right)^{-1}\left(\mathbf{1}-\hat{U}\right),$$

with $A$ a self-adjoint $2\times 2$ matrix. By allowing some entries of $A$ that take the value $\infty$, it is possible to recover some cases $\left(\mathbf{1}+\hat{U}\right)$ that are not invertible; nevertheless, it is not always a simple task to recover all such cases, so that the boundary conditions in terms of $\hat{U}$ seem preferable.

*Exercise* 7.3.5. Show that $A$ above is actually a self-adjoint matrix. Note that it recalls the inverse Cayley transform.

*Exercise* 7.3.6. Check that the choices for the matrix $\hat{U}$

$$\text{a) } \mathbf{1}, \qquad \text{b) } -\mathbf{1}, \qquad \text{c) } \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \text{d) } \begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix},$$

impose, respectively, the boundary conditions: a) $\psi(0) = 0 = \psi(1)$ (Dirichlet); b) $\psi'(0) = 0 = \psi'(1)$ (Neumann); c) $\psi(0) = \psi(1)$ and $\psi'(0) = \psi'(1)$ (periodic); d) $\psi(0) = -\psi(1)$ and $\psi'(0) = -\psi'(1)$ (antiperiodic).

*Exercise* 7.3.7. With respect to Exercise 7.3.6, find the spectra of all those operators by solving the corresponding eigenvalue equations; confirm that they are formed solely of eigenvalues. Check that cases a) and b) have the same spectra, except for $E = 0$ that is an eigenvalue only in case b) and, in both cases, all eigenvalues are simple. Note that the multiplicity of all eigenvalues in case d) is two.

*Example* 7.3.8. If the potential $V$ is such that both end points $0, 1$ are regular, then the deficiency indices of $H\psi = -\psi'' + V\psi$, dom $H = C_0^\infty(0,1)$, are equal to 2, and for any $\psi \in$ dom $H^*$ the boundary values $\psi(0), \psi(1), \psi'(0), \psi'(1)$ are well defined. Thus, its self-adjoint extensions can be characterized in the same way as in Example 7.3.4, through the same boundary conditions. Particular cases are

$$V(x) = \kappa \ln x, \qquad V(x) = \kappa/x^\alpha, \qquad \alpha < 1,\ \kappa \in \mathbb{R}.$$

*Example* 7.3.9. Let $V(x)$ be continuous and lower bounded with $|V(x)| \le |x|^{-\alpha}$, for some $0 < \alpha < 1/2$, and $H\psi = -\psi'' + V\psi$, dom $H = C_0^\infty(\mathbb{R})$. By Theorem 6.2.23, $H$ is in the limit point case at both end points $-\infty, +\infty$, so that $H^*$ is self-adjoint, with dom $H^* = \mathcal{H}^2(\mathbb{R})$ and $H^*\psi = -\psi'' + V\psi$.

## 7.4 Singular Examples and All That

For singular endpoints the limit values of $\psi, \psi'$ could not exist, so that the strategy presented in the examples in Section 7.3 is not guaranteed to work. However, in some cases it is possible to properly adapt that strategy in order to get self-adjoint extensions. This will be illustrated in this section through a series of examples, including some point interactions.

*Example* 7.4.1. The self-adjoint extensions of $\mathrm{dom}\, H = C_0^\infty(0,1)$,

$$(H\psi)(x) = -\psi''(x) - \frac{1}{4x^2}\psi(x), \qquad \psi \in \mathrm{dom}\, H,$$

will be found (cf., Example 7.2.18 and Exercise 7.2.23). If $\psi \in \mathrm{dom}\, H^* = \{\psi \in \mathrm{L}^2(0,1) : \psi, \psi' \in \mathrm{AC}(0,1), (-\psi'' - \psi/(4x^2)) \in \mathrm{L}^2(0,1)\}$ one has

$$u = H^*\psi = -\psi'' - \frac{1}{4x^2}\psi \in \mathrm{L}^2(0,1),$$

which is a nonhomogeneous second-order linear differential equation for $\psi$; the general solution of the corresponding homogeneous equation $H^*\psi = 0$ is $b_1\psi_1(x) + b_2\psi_2(x)$, $b_1, b_2 \in \mathbb{C}$, with $\psi_1(x) = \sqrt{x}$ and $\psi_2(x) = \sqrt{x}\,\ln x$, whose wronskian is $W_x[\overline{\psi_1}, \psi_2] = 1$, $\forall x \in [0,1]$. Introduce $\varphi = \psi/\sqrt{x}$ so that

$$\sqrt{x}\,\varphi'' + \frac{1}{\sqrt{x}}\varphi' = -u,$$

or

$$(x\varphi')' = x\varphi'' + \varphi' = -\sqrt{x}u,$$

and since $\sqrt{x}u \in \mathrm{L}^1[0,1]$, on integrating one gets

$$\varphi'(x) = \frac{b_2}{x} - \frac{1}{x}\int_0^x \sqrt{s}\,u(s)\,ds.$$

By Cauchy-Schwarz, the function $x \mapsto \frac{1}{x}\int_0^x \sqrt{s}u(s)\,ds$ is also integrable in $[0,1]$, so that

$$\varphi(x) = b_1 + b_2 \ln x - \int_0^x \frac{ds}{s}\int_0^s \sqrt{t}\,u(t)\,dt$$

and, finally, $\psi(x) = b_1\sqrt{x} + b_2\sqrt{x}\,\ln x + v_\psi(x)$, (note that $b_j = b_j(\psi)$, $j = 1,2$) with $v_\psi$ denoting the differentiable function

$$v_\psi(x) = -\sqrt{x}\int_0^x \frac{ds}{s}\int_0^s \sqrt{t}\,u(t)\,dt.$$

By Cauchy-Schwarz again,

$$\begin{aligned} |v_\psi(x)| &\le \sqrt{x}\int_0^x \frac{ds}{s}\left|\int_0^s \sqrt{t}\,u(t)\right| dt \\ &\le \sqrt{x}\int_0^x \frac{ds}{s}\frac{s}{\sqrt{2}}\,\|u\|_2 = \frac{x^{3/2}}{\sqrt{2}}\,\|u\|_2, \end{aligned}$$

so that $v_\psi(x) \sim x^{3/2}$, $v_\psi'(x) \sim x^{1/2}$ as $x \to 0$.

The boundary form of $H$ is, for $\psi, \varphi \in \text{dom } H^*$,

$$\psi(x) = b_1(\psi)\sqrt{x} + b_2(\psi)\sqrt{x}\,\ln x + v_\psi(x)$$

and

$$\varphi(x) = b_1(\varphi)\sqrt{x} + b_2(\varphi)\sqrt{x}\,\ln x + v_\varphi(x),$$

$$\begin{aligned}\Gamma(\psi,\varphi) &= W_1[\psi,\varphi] - W_0[\psi,\varphi] \\ &= \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) + \lim_{x\to 0^+}\left(-\overline{\psi(x)}\varphi'(x) + \overline{\psi'(x)}\varphi(x)\right) \\ &= \overline{\psi(1)}\varphi'(1) - \overline{\psi'(1)}\varphi(1) - \overline{b_1(\psi)}b_2(\varphi) + b_1(\varphi)\overline{b_2(\psi)}.\end{aligned}$$

*Remark* 7.4.2. The above procedure, to deal with functions in dom $H^*$, was an alternative to the use of the variation of parameters formula employed in Example 7.2.18.

Based on Example 7.3.1, define the two-dimensional vector spaces of elements

$$\Psi = \begin{pmatrix} b_2(\psi) - ib_1(\psi) \\ \psi'(1) + i\psi(1) \end{pmatrix}, \qquad \rho(\Psi) = \begin{pmatrix} b_2(\psi) + ib_1(\psi) \\ \psi'(1) - i\psi(1) \end{pmatrix},$$

for $\psi \in \text{dom } H^*$. A direct evaluation of inner products leads to

$$\langle \Psi, \Phi\rangle - \langle \rho(\Psi), \rho(\Phi)\rangle = -2i\Gamma(\psi,\varphi),$$

and a boundary triple for $H$ was found. The self-adjoint extensions $H_{\hat{U}}$ of $H$ are associated with $2\times 2$ unitary matrices $\hat{U}$ that entail the boundary conditions

$$\left(\mathbf{1} - \hat{U}\right)\begin{pmatrix} b_2(\psi) \\ \psi'(1) \end{pmatrix} = -i\left(\mathbf{1} + \hat{U}\right)\begin{pmatrix} -b_1(\psi) \\ \psi(1) \end{pmatrix},$$

that is, the domain of the self-adjoint extension $H_{\hat{U}}$ of $H$ is composed of the elements $\psi \in \text{dom } H^*$ so that the above boundary conditions are satisfied; also $H_{\hat{U}}\psi = H^*\psi$, $\forall \psi \in \text{dom } H_{\hat{U}}$. The reader can play with different choices of $\hat{U}$ in order to get explicit self-adjoint extensions. What about some with $b_2 = 0$?

### 7.4.1 One-dimensional H-Atom

The operator with domain dom $H = C_0^\infty(\mathbb{R}\setminus\{0\})$ and action

$$H = -d^2/dx^2 - \kappa/|x|, \qquad \kappa > 0, \quad x \in \mathbb{R}\setminus\{0\},$$

is known as the (initial) one-dimensional hydrogen atom hamiltonian. It easily follows that $H$ is hermitian and the question is to determine its self-adjoint extensions. In the way of finding such extensions, some typical difficulties encountered when dealing with more realistic potentials will appear. This model has a controversial history which can be traced through the references in the article [LoCdO06].

First the deficiency indices will be handled. Write

$$C_0^\infty(\mathbb{R} \setminus \{0\}) = C_0^\infty(-\infty, 0) \oplus C_0^\infty(0, \infty)$$

and set $H_1 = H|_{C_0^\infty(-\infty,0)}$ and $H_2 = H|_{C_0^\infty(0,\infty)}$, so that $H = H_1 \oplus H_2$. By Proposition 2.3.20, dom $H_1^* = \{\psi \in \mathrm{L}^2(-\infty, 0) : \psi, \psi' \in \mathrm{AC}(-\infty, 0), (-\psi'' - \kappa/|x|\psi) \in \mathrm{L}^2(-\infty, 0)\}$, dom $H_2^* = \{\psi \in \mathrm{L}^2(0, \infty) : \psi, \psi' \in \mathrm{AC}(0, \infty), (-\psi'' - \kappa/|x|\psi) \in \mathrm{L}^2(0, \infty)\}$ and

$$(H_j^*\psi)(x) = -\psi''(x) - \frac{\kappa}{|x|}\psi(x), \qquad \psi \in \mathrm{dom}\ H_j^*, \quad j = 1, 2.$$

Hence, dom $H^* = \{\psi \in \mathrm{L}^2(\mathbb{R}) : \psi, \psi' \in \mathrm{AC}(\mathbb{R} \setminus \{0\}), (-\psi'' - \kappa/|x|\psi) \in \mathrm{L}^2(\mathbb{R})\}$ and $H^*$ with the same action as $H$.

By using Whittaker functions [GraR80] (solutions of a particular confluent hypergeometric equation) in [Mos93] it was shown that for $\psi \in \mathrm{dom}\ H^*$ the lateral limits $\psi(0^\pm) := \lim_{x\to 0^\pm} \psi(x)$ are finite while $\psi'(x)$ has logarithmic divergences as $x \to 0^\pm$. Furthermore, $\lim_{x\to\pm\infty} \psi(x) = 0$, $\lim_{x\to\pm\infty} \psi'(x) = 0$. With such information, a characterization of $\psi'(0^\pm)$ is possible. The following lemma is an alternative way of getting such information.

**Lemma 7.4.3.** *If* $\psi \in \mathrm{dom}\ H^*$*, then the lateral limits* $\psi(0^\pm) = \lim_{x\to 0^\pm} \psi(x)$ *and*

$$\tilde{\psi}(0^\pm) := \lim_{x\to 0^\pm} (\psi'(x) \pm \kappa\psi(x) \ln(|\kappa x|))$$

*exist and are finite.*

*Proof.* We will discuss the case $x > 0$; the other $x < 0$ is similar. For $\psi \in \mathrm{dom}\ H^*$ one has

$$-H^*\psi = \frac{d^2\psi}{dx^2} + \frac{\kappa}{x}\psi := u \in \mathrm{L}^2(0, \infty),$$

and one can write $\psi = \psi_1 + \psi_2$ with $\psi_1'' = u$, $\psi_1(0^+) = 0$ and $\psi_2'' + \kappa/x\psi = 0$. Since $\psi_j \in \mathcal{H}^2(\varepsilon, \infty)$, $j = 1, 2$, for all $\varepsilon > 0$, and $u \in \mathrm{L}^2$, it follows that these functions are of class $C^1(0, \infty)$.

Consider an interval $[x, c]$, $0 < x < c < \infty$; $c$ will be fixed later on. Since

$$\psi_1'(x) - \psi_1'(c) = \int_x^c u(s)\, ds,$$

$\psi_1'(x)$ has a lateral limit

$$\psi_1'(0^+) = \psi'(c) + \int_0^c u(s)\, ds.$$

On integrating successively twice over the interval $[x, c]$ one gets

$$\psi_2'(c) - \psi_2'(x) = -\kappa \int_x^c \frac{\psi(s)}{s}\, ds,$$

and then

$$\psi_2(x) = \psi_2(c) - (c-x)\psi_2'(c) - \kappa \int_x^c dv \int_v^c ds\, \frac{\psi(s)}{s}$$
$$= \psi_2(c) - (c-x)\psi_2'(c) - \kappa \int_x^c ds\, \psi(s)\, \frac{s-x}{s},$$

and since $0 \le (s-x)/s < 1$, by dominated convergence the last integral converges to $\int_0^1 \psi(s)$ as $x \to 0^+$. Therefore $\psi_2(0^+)$ exists and

$$\psi_2(0^+) = \psi_2(c) - c\psi_2'(c) - \kappa \int_0^c \psi(s)\, ds.$$

Now,

$$\left|\psi_2(x) - \psi_2(0^+)\right| \le x|\psi_2'(c)| + \kappa \int_0^x |\psi(s)|\, ds + \kappa x \int_x^c ds\, \frac{|\psi(s)|}{s}.$$

Taking into account that $\psi$ is bounded, say $|\psi(x)| \le C$, $\forall x$, Cauchy-Schwarz in $\mathrm{L}^2$ implies

$$\int_0^x |\psi(s)| ds = \int_0^x 1\, |\psi(s)| ds \le C\sqrt{x},$$

and so, for $0 < x$ small enough and fixing $c = 1$,

$$\int_x^c ds \frac{\psi(s)}{s} \le C\left(c|\ln c| + x|\ln x|\right) \le \tilde{C}\sqrt{x},$$

for some constant $\tilde{C}$. Such inequalities imply $\psi(x) = \psi(0^+) + O(\sqrt{x})$, and on substituting this into

$$\psi'(x) = \psi'(1) + \kappa \int_x^1 \frac{\psi(s)}{s}\, ds$$

(recall that $\psi_1'(0^+)$ is finite) it is found that there is $b$ so that, as $x \to 0^+$,

$$\psi'(x) = \psi'(1) - \kappa\psi(0^+) \ln(\kappa x) + b + o(1);$$

thus, the derivative $\psi'$ has a logarithmic divergence as $r \to 0$ and the statement in the lemma also follows. □

By means of Whittaker's functions [Mos93] one gets the values $n_-(H_1) = 1 = n_+(H_1)$ and $n_-(H_2) = 1 = n_+(H_2)$, so that $n_-(H) = 2 = n_+(H)$. Similarly to Example 7.3.4, taking into account that $\psi, \psi'$ vanish at $\pm\infty$, it follows that

$$\Gamma(\psi, \varphi) = W_{0^+}[\psi, \varphi] - W_{0^-}[\psi, \varphi]$$
$$= \lim_{x \to 0^+} \left(\overline{\psi(x)}\varphi'(x) - \overline{\psi'(x)}\varphi(x)\right) + \lim_{x \to 0^-} \left(\overline{\psi'(x)}\varphi(x) - \overline{\psi(x)}\varphi'(x)\right).$$

Though the right-hand side is finite, each lateral limit may diverge. However, invoking Lemma 7.4.3 and since one readily checks that

$$\Gamma(\psi,\varphi) = \overline{\psi(0^+)}\tilde{\varphi}(0^+) - \overline{\tilde{\psi}(0^+)}\varphi(0^+) + \overline{\tilde{\psi}(0^-)}\varphi(0^-) - \overline{\psi(0^-)}\tilde{\varphi}(0^-),$$

but now each lateral limit is finite, again by following Example 7.3.4 a boundary triple was constructed. The self-adjoint extensions $H_{\hat{U}}$ of $H$ are associated with $2\times 2$ unitary matrices $\hat{U}$ that entail the boundary conditions

$$\left(\mathbf{1} - \hat{U}\right)\begin{pmatrix}\tilde{\psi}(0^-)\\ \tilde{\psi}(0^+)\end{pmatrix} = -i\left(\mathbf{1} + \hat{U}\right)\begin{pmatrix}-\psi(0^-)\\ \psi(0^+)\end{pmatrix},$$

and the domain of the self-adjoint extension $H_{\hat{U}}$ of $H$ is composed of the elements $\psi \in \operatorname{dom} H^*$ so that the above boundary conditions are satisfied; also $H_{\hat{U}}\psi = H^*\psi$. Dirichlet boundary conditions $\psi(0^-) = 0 = \psi(0^+)$ are obtained by choosing $\hat{U} = \mathbf{1}$. Some boundary conditions mix the right and left half-lines, which are interpreted as quantum permeability of the singularity at the origin, that is, the particle is allowed to pass through the origin; see more details in Exercise 14.4.10 and [deOV08]. The above discussion also holds for $\kappa < 0$.

*Exercise* 7.4.4. Based on the arguments used to conclude Corollary 7.2.5, find the closure of the initial operator for the one-dimensional H-atom, that is, $H = -d^2/dx^2 - \kappa/|x|$ with domain $C_0^\infty(\mathbb{R}\setminus\{0\})$.

## 7.4.2 Some Point Interactions

Roughly speaking, *point interactions* are a kind of potential concentrated on a single point of $\mathbb{R}^n$, which are also called *zero-range potentials* and *delta-function potentials*. Often they are properly defined via the choice of domains and boundary conditions at the point in question, and it is a possible way to describe a hamiltonian with a Dirac $\delta$ potential.

Physically, the main consequence of extracting a point of $\mathbb{R}^n$ is that translation invariance is lost, which has impressive consequences on some quantum observables (i.e., operators) since the unique self-adjointness can also be lost (at least in dimensions $n \le 3$).

Different approaches for associating self-adjoint operators to point interactions are discussed in [Zor80]; more information can be obtained from the books [AGKH05] and [AlK00]. In those references, in case of $\mathbb{R}^n$, $n \le 3$, self-adjoint extensions of hermitian (Schrödinger) operators with point interactions are characterized and their spectral properties explicitly computed. Hence, point interactions have been called "solvable models" and used to approximately study physical systems with "very short range" potentials.

Here a few of the simplest cases will be discussed; Example 4.4.9 can be considered the first instance of point interaction in this book.

*Example* 7.4.5. Let $T = -id/dx$ with

$$\mathrm{dom}\ T = C_0^\infty(\mathbb{R} \setminus \{0\}) = C_0^\infty(-\infty, 0) \oplus C_0^\infty(0, \infty).$$

One point was removed and the self-adjoint extensions are obtained from dom $T^*$ through suitable matching conditions at the origin (recall that in case the domain is $C_0^\infty(\mathbb{R})$ the operator $T$ is essentially self-adjoint; see Section 3.3). Set $T_1 = T|_{C_0^\infty(-\infty,0)}$ and $T_2 = T|_{C_0^\infty(0,\infty)}$, so that $T = T_1 \oplus T_2$. One has dom $T^* = \{\psi \in \mathrm{AC}(\mathbb{R} \setminus \{0\}) : \psi' \in \mathrm{L}^2(\mathbb{R})\}$, $T^*\psi = -i\psi'$.

*Exercise* 7.4.6. Check that

$$\mathrm{dom}\ T_1^* = \{\psi \in \mathrm{AC}(-\infty, 0) : \psi' \in \mathrm{L}^2(-\infty, 0]\},$$
$$\mathrm{dom}\ T_2^* = \{\psi \in \mathrm{AC}(0, \infty) : \psi' \in \mathrm{L}^2[0, \infty)\},$$

and verify that $T^*$ is the above operator.

In order to determine the deficiency indices consider the $\mathrm{K}_\pm$-equations

$$(T_2^* \pm i\mathbf{1})\psi_\pm = 0,$$

whose solutions are proportional to $\psi_\pm(x) = e^{\pm x}$. Similarly for $T_1$. Hence $n_-(T_1) = 0 = n_+(T_2)$, $n_-(T_2) = 1 = n_+(T_1)$, and combining these values one obtains $n_-(T) = 1 = n_+(T)$.

*Exercise* 7.4.7. Follow the proof of Lemma 7.4.3 to show that, for $\psi \in$ dom $T^*$, the lateral limits $\psi(0^-), \psi(0^+)$, exist.

Now, for $\psi, \varphi \in$ dom $T^*$ the boundary form is found (on integrating by parts):

$$\begin{aligned}\Gamma(\psi, \varphi) &= \langle T^*\psi, \varphi\rangle - \langle \psi, T^*\varphi\rangle \\ &= \left(\int_{-\infty}^{0^-} + \int_{0^+}^{\infty}\right) dx\ \left((\overline{-i\psi'(x)})\varphi(x) - \overline{\psi(x)}(-i\varphi'(x))\right) \\ &= i\left(\overline{\psi(0^+)}\varphi(0^+) - \overline{\psi(0^-)}\varphi(0^-)\right).\end{aligned}$$

Introduce the one-dimensional vector spaces $X = \{\psi(0^+) : \psi \in \mathrm{dom}\ T^*\}$ and $Y = \{\psi(0^-) = \rho(\psi(0^+) : \psi \in \mathrm{dom}\ T^*\}$ and note that $\Gamma(\psi, \varphi) = 0$ is equivalent to the equality of inner products

$$\langle \psi(0^+), \varphi(0^+)\rangle = \langle \rho(\psi(0^+)), \rho(\varphi(0^+))\rangle.$$

Self-adjoint extensions are obtained on domains $\mathcal{D} \subset$ dom $T^*$ so that $\Gamma(\psi, \varphi) = 0$, $\forall \psi, \varphi \in \mathcal{D}$, that is, $X$ and $Y$ are related by unitary maps $e^{i\theta}$, $0 \le \theta < 2\pi$; explicitly $\psi(0^+) = e^{i\theta}\psi(0^-)$.

Therefore, the family of operators

$$\mathrm{dom}\ T_\theta = \left\{\psi \in \mathrm{AC}(\mathbb{R} \setminus \{0\}) : \psi' \in \mathrm{L}^2(\mathbb{R}), \psi(0^+) = e^{i\theta}\psi(0^-)\right\},$$
$$T_\theta \psi = -i\frac{d\psi}{dx},$$

constitutes the self-adjoint extensions of $T$. The case $\theta = 0$ agrees with the momentum operator $P$ (see Example 2.3.11 and Section 3.3) defined without point interaction, that is, with initial domain $C_0^\infty(\mathbb{R})$.

*Exercise* 7.4.8. Find the self-adjoint extensions of the hermitian operator dom $T = C_0^\infty(\mathbb{R} \setminus \{0\})$, $T\psi = -\psi''$. Show that its deficiency indices are $n_- = n_+ = 2$.

*Exercise* 7.4.9. A circumference with one point removed can be considered a segment, say $[0,1]$, with the ends identified. Write $0 = 0^+$ and $1 = 0^-$, and construct the possible hamiltonians of a free particle on this circumference as self-adjoint extensions of dom $H = C_0^\infty(0^+, 0^-)$, $H\psi = -\psi''$.

*Example* 7.4.10. This should be compared with Example 7.4.5. It is another possible way to define self-adjoint realizations of $T = -i\frac{d}{dx}$ in $\mathrm{L}^2(\mathbb{R})$ with the origin removed. Here one takes dom $T = \{\psi \in \mathcal{H}^1(\mathbb{R}) : \psi(0) = 0\}$. It also illustrates another way of finding self-adjoint extensions. By using Fourier transform, this operator (see Section 3.3) is rewritten as a specific multiplication operator $S = \mathcal{F}^{-1}T\mathcal{F}$ so that

$$\mathrm{dom}\ S = \left\{\phi \in \mathrm{dom}\ P = \mathcal{H}^1(\hat{\mathbb{R}}) : 0 = \int_{\mathbb{R}} \phi(p)\, dp\right\}, \quad (S\phi)(p) = p\phi(p).$$

Recall that for $\psi \in \mathcal{H}^1(\mathbb{R})$ one has $\psi(0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{\psi}(p)\, dp$, whose integral means $\lim_{M\to\infty} \int_{-M}^{M} \hat{\psi}(p)\, dp$; this explains dom $S$.

*Exercise* 7.4.11. Show that $S$ (and so $T$) is a hermitian operator.

*Lemma* 7.4.12. a) *$S$ is a closed operator.*

b) *The solutions $u \in \mathrm{L}^2_{\mathrm{loc}}(\hat{\mathbb{R}})$ (or $\mathrm{L}^1_{\mathrm{loc}}(\hat{\mathbb{R}})$) of $\int_{\mathbb{R}} \phi(p)u(p)\, dp = 0$, $\forall \phi \in$ dom $S$, are the constant functions.*

*Proof.* a) Let $\psi_n \to \psi$ and $S\psi_n \to \phi$, $\psi_n \in$ dom $S$. For each $M > 0$ one has $\|\psi_n - \psi\| < 1/M$ if $n$ is large enough. By Cauchy-Schwarz,

$$\left|\int_{-M}^{M} (\psi - \psi_n)\, dx\right| \le (2M)^{1/2} \|\psi_n - \psi\| < \sqrt{\frac{2}{M}}.$$

Since $\int_{\mathbb{R}} \psi_n\, dx = 0$, $\forall n$, choose $n$ so that $\left|\int_{-M}^{M} \psi_n\, dx\right| < \sqrt{2/M}$; thus

$$\left|\int_{-M}^{M} \psi\, dx\right| \le \left|\int_{-M}^{M} (\psi - \psi_n)\, dx\right| + \left|\int_{-M}^{M} \psi_n\, dx\right| < 2\sqrt{\frac{2}{M}}$$

and it follows that $\int_{\mathbb{R}} \psi\, dx = 0$. Denote $|||\varphi|||_M := \left(\int_M^M |\varphi|^2\, dx\right)^{1/2}$. Pick $n$ so large that $\|S\psi_n - \phi\| < 1/M^{1/2}$, and $\|\psi - \psi_n\| < 1/M$; then

$$\begin{aligned} |||p\psi|||_M &\le |||p(\psi - \psi_n)|||_M + |||p\psi_n - \phi|||_M + |||\phi|||_M \\ &\le M^{1/2} |||\psi - \psi_n|||_M + |||S\psi_n - \phi|||_M + \|\phi\| \\ &\le M^{1/2} \|\psi - \psi_n\| + \|S\psi_n - \phi\| + \|\phi\| < \frac{2}{M^{1/2}} + \|\phi\|, \end{aligned}$$

and for $M \to \infty$ one obtains $\|S\psi\| \le \|\phi\|$, consequently $\psi \in \text{dom } S$. Similarly, by picking $n$ large enough so that $\|\psi - \psi_n\| < 1/M$ and $\|S\psi_n - \phi\| < 1/M^{1/2}$, one gets

$$\begin{aligned}|||S\psi - \phi|||_M &\le |||S\psi - S\psi_n|||_M + |||S\psi_n - \phi|||_M \\ &\le M^{1/2}\|\psi - \psi_n\| + \|S\psi_n - \phi\| < \frac{2}{M^{1/2}}.\end{aligned}$$

Therefore $S\psi = \phi$ and $S$ is a closed operator.

b) Note that the problem has no nonzero solution $u \in \mathrm{L}^2(\hat{\mathbb{R}})$, since such $u$ would be orthogonal to the dense set dom $S$. Further, dom $S$ contains the derivative $\phi'$ of all $\phi \in C_0^\infty(\mathbb{R})$ (since $\int \phi'\, dx = 0$), and so the distributional derivative $u'$ of any solution $u$ is null; the result then follows by applying Lemma 2.3.9. ☐

The deficiency spaces are $\mathrm{K}_\pm(S) = \text{rng } (S \mp i\mathbf{1})^\perp$. Thus, for $u_\pm \in \mathrm{K}_\pm(S)$ one has, for all $\phi \in \text{dom } S$,

$$\begin{aligned}0 &= \langle (S \mp i\mathbf{1})\phi, u_\pm\rangle = \int_{\mathbb{R}} \overline{(p \mp i)\phi(p)}\, u_\pm(p)\, dp \\ &= \int_{\mathbb{R}} \overline{\phi(p)}\, (p \pm i) u_\pm(p)\, dp \Longrightarrow u_\pm(p) = \frac{1}{p \pm i}.\end{aligned}$$

Lemma 7.4.12 was employed and, actually, the above $u_\pm$ linearly spans $\mathrm{K}_\pm(S)$, so that $n_- = n_+ = 1$; note that $\|u_-\| = \|u_+\|$. Thus the self-adjoint extensions $S_\theta$ of $S$ are parametrized by $e^{i\theta}$, $0 \le \theta < 2\pi$, and given by (see Proposition 2.5.8)

$$\begin{aligned}\text{dom } S_\theta &= \{\phi_\theta = \phi + c(u_- - e^{i\theta}u_+) : \phi \in \text{dom } S, c \in \mathbb{C}\}, \\ (S_\theta\phi_\theta)(p) &= p\phi(p) + ci\left(u_-(p) + e^{i\theta}u_+(p)\right).\end{aligned}$$

By recalling of Section 3.3, the following question naturally arises: For which values of $\theta$ do $S_\theta$ act as multiplication by $p$? Since $u_\pm(p) = 1/(p \pm i)$ one has

$$S_\theta(u_- - e^{i\theta}u_+)(p) = i\frac{p(1 + e^{i\theta}) + i(1 - e^{i\theta})}{1 + p^2},$$

and by imposing that it equals $p(u_- - e^{i\theta}u_+)(p)$, it follows that $\theta = 0$. Surely $S_0$ corresponds to the usual multiplication operator $\mathcal{M}_p$ acting in $\mathrm{L}^2(\hat{\mathbb{R}})$, which is the usual momentum operator $P$ (see Example 2.3.11 and Section 3.3), clearly a self-adjoint extension of $T$.

*Exercise* 7.4.13. Apply the procedure in Example 7.4.10 to find all self-adjoint extensions of $T\psi = -\Delta\psi$, dom $T = \{\psi \in \mathcal{H}^2(\mathbb{R}^n) : \psi(0) = 0\}$, for $n \in \mathbb{N}$. Note that there is a problem for $n \ge 4$, since by Sobolev embedding the functions in dom $T$ are not ensured to be continuous; in any event, for all $n$ the following operators obtained after Fourier transforming are well defined:

$$\text{dom } S = \left\{\phi \in \text{dom } P : 0 = \int_{\mathbb{R}^n} \phi(p)\, dp\right\}, \qquad (S\phi)(p) = p^2\phi(p).$$

What is it possible to conclude about the operator $S$ for $n \geq 4$? See Remark 7.4.14 for related issues.

*Remark* 7.4.14. In [Far75], page 33, it is shown that the set $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ is dense in $\mathcal{H}^2(\mathbb{R}^n)$ iff $n \geq 4$. From this it follows that $\dot{H} = -\Delta$, dom $\dot{H} = C_0^\infty(\mathbb{R}^n \setminus \{0\})$, is essentially self-adjoint iff $n \geq 4$, and in this case its unique self-adjoint extension is $H_0 = -\Delta$, dom $H_0 = \mathcal{H}^2(\mathbb{R}^n)$. As a matter of fact, clearly $H_0$ is a self-adjoint extension of $\dot{H}$, and since the graph norm of $H_0$ is equivalent to the norm of $\mathcal{H}^2(\mathbb{R}^n)$, $C_0^\infty(\mathbb{R}^n \setminus \{0\})$ is a core of $H_0$ iff this set is dense in $\mathcal{H}^2(\mathbb{R}^n)$; so, iff $n \geq 4$.

*Remark* 7.4.15. The procedures discussed in Examples 7.4.5 and 7.4.10 to remove the origin are not equivalent in general. When applied to the operator $T\psi = -\psi''$ in $\mathbb{R}$ (see Exercises 7.4.8 and 7.4.13), the former procedure results in deficiency indices $n_- = 2 = n_+$, whereas the latter in $n_- = 1 = n_+$.

## 7.5 Spherically Symmetric Potentials

A potential $v : \mathbb{R}^n \to \mathbb{R}$ is *spherically symmetric* (also called *radial* or *central*) if its values depend only on $r = |x|$, that is, if there exists $V : [0, \infty) \to \mathbb{R}$ so that $v(x) = V(r)$.

It is convenient to exclude the origin and take as the initial hamiltonian operator

$$H = -\Delta + V(r), \qquad \text{dom } H = C_0^\infty(\mathbb{R}^n \setminus \{0\}).$$

It is natural to introduce the radius $r$ and $n-1$ angle variables $\Omega = \{\omega_1, \ldots, \omega_{n-1}\}$ for the description of the system. For instance, if $n = 3$ one passes from cartesian $x = (x_1, x_2, x_3)$ to spherical $(r, \varphi, \theta)$ coordinates $x_1 = r \sin\theta \cos\varphi$, $x_2 = r \sin\theta \cos\varphi$, $x_3 = r\cos\theta$, so that $\mathrm{L}^2(\mathbb{R}^3)$ is unitarily equivalent to

$$E^3 = \mathrm{L}^2_{r^2 dr}([0, \infty)) \otimes \mathrm{L}^2_{d\Omega}(S^2),$$

with $S^2$ denoting the unit sphere in $\mathbb{R}^3$ and $d\Omega = \sin\theta d\theta d\varphi$. If $n = 2$ polar coordinates $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$ are introduced so that $\mathrm{L}^2(\mathbb{R}^2)$ is unitarily equivalent to

$$E^2 = \mathrm{L}^2_{rdr}([0, \infty)) \otimes \mathrm{L}^2_{d\varphi}(S^1),$$

with $S^1$ denoting the unit circumference in $\mathbb{R}^2$. Here only $n = 2, 3$ will be considered, although many results have straight counterparts in higher dimensions; see, e.g., [Mu66].

By Lemma 1.4.8 the set of finite linear combinations of the functions $R(r)\Phi(\theta, \varphi) \in E^3$ (resp. $R(r)\Phi(\varphi) \in E^2$) is dense in $\mathrm{L}^2(\mathbb{R}^3)$ (resp. $\mathrm{L}^2(\mathbb{R}^2)$) and the spherical harmonics $Y_{lm}(\theta, \varphi)$, $l \in \mathbb{N} \cup \{0\}$, $-l \leq m \leq l$, (resp. $e_m(\varphi) = e^{im\varphi}/\sqrt{2\pi}$, $m \in \mathbb{Z}$) form an orthonormal basis of $\mathrm{L}^2(S^2)$ (resp. $\mathrm{L}^2(S^1)$). For functions $R(r)Y_{lm}(\theta, \varphi)$, $R \in C_0^\infty(0, \infty)$, in case $n = 3$, the well-known expression of the laplacian $\Delta$ in spherical coordinates implies that (see, e.g., [Will03])

$$H(RY_{lm}) = \left( -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} + V(r) \right) RY_{lm},$$

and after the unitary transformation $u_3 : \mathrm{L}^2_{r^2dr}([0,\infty)) \to \mathrm{L}^2_{dr}([0,\infty))$, $(u_3R)(r) = rR(r)$, one obtains for $u_3Hu_3^{-1}$ restricted to the subspace spanned by $Y_{lm}$ (note that $u_3(C_0^\infty(0,\infty)) \subset C_0^\infty(0,\infty)$)

$$\hat{H}_{lm} = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r), \qquad \mathrm{dom}\ \hat{H}_{lm} = C_0^\infty(0,\infty).$$

For $n = 2$ one has

$$H(Re_m) = \left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2} + V(r)\right) Re_m,$$

and after the unitary transformation $u_2 : \mathrm{L}^2_{rdr}([0,\infty)) \to \mathrm{L}^2_{dr}([0,\infty))$, with $(u_2R)(r) = \sqrt{r}R(r)$, one obtains for $u_2Hu_2^{-1}$ restricted to the subspace spanned by $e_m$,

$$\hat{H}_m = -\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{r^2} + V(r), \qquad \mathrm{dom}\ \hat{H}_m = C_0^\infty(0,\infty).$$

In both cases, i.e., $n = 2, 3$, the original problem is reduced to the study of infinitely many Schrödinger operators on the half-line $[0,\infty)$ with suitable effective potentials $\hat{V}_m$ or $\hat{V}_{l,m}$; e.g., in the two-dimensional case,

$$\hat{V}_m(r) = (m^2 - 1/4)/r^2 + V(r), \qquad m \in \mathbb{Z}.$$

The previous discussions in this chapter, about Schrödinger operators on intervals, apply to $\hat{H}_m$ and $\hat{H}_{lm}$.

*Remark* 7.5.1. Note that the *radial momentum operator* $-id/dr$ is not defined as a physical quantity on $C_0^\infty(0,\infty)$, since it has no self-adjoint extensions (see Example 2.3.17 and an intuitive digression in Remark 5.4.7).

*Exercise* 7.5.2. Consider $\hat{H}_{lm}$ and $\hat{H}_m$ in $\mathbb{R}^3$ and $\mathbb{R}^2$, respectively, for the free particle, i.e., $V = 0$ identically. Use results of this chapter to show that $\hat{H}_{lm}$ (resp. $\hat{H}_m$) is not essentially self-adjoint only if $l = 0$ (resp. $m = 0$). Find the corresponding deficiency indices. What can be said about $H = -\Delta$, $\mathrm{dom}\ H = C_0^\infty(\mathbb{R}^n \setminus \{0\})$, $n = 2, 3$? Cf. Exercise 7.4.8.

Now some particular cases of minimal operators $\mathrm{dom}\ H = C_0^\infty(0,\infty)$, $H\psi = -\psi'' + V(r)\psi$ will be discussed (think of the above notation with $\hat{V}$ replaced by $V$). In the remainder of this section, $H$ always denotes this operator.

**Proposition 7.5.3.** *If* $V \in \mathrm{L}^2(0,\infty)$, *then* $n_-(H) = 1 = n_+(H)$ *and*

$$\Gamma_{H^*}(\psi,\varphi) = -W_0[\psi,\varphi], \qquad \forall \psi,\varphi \in \mathrm{dom}\ H^*.$$

**Lemma 7.5.4.** *Fix* $c > 0$. *If* $V \in \mathrm{L}^2(0,\infty)$, *then for each* $\psi \in \mathrm{dom}\ H^*$ *there exists* $0 \le C < \infty$ *so that*

$$\left|\frac{\psi'(x)}{\sqrt{x}}\right| \le C, \qquad \forall x > c.$$

*Proof.* For $\psi \in \operatorname{dom} H^*$ one has $-\psi'' + V\psi = u \in \mathrm{L}^2(0,\infty)$; integrating $u$ and taking into account that $V\psi \in \mathrm{L}^1(0,\infty)$ one obtains ($x > c$)

$$\psi'(x) = \psi'(c) + \int_c^x dt\, V(t)\psi(t) - \int_c^x dt\, u(t),$$

and by Cauchy-Schwarz,

$$\begin{aligned} |\psi'(x)| &\le |\psi'(c)| + \int_c^x dt\, |V(t)\psi(t)| + \int_c^x dt\, |u(t)| \\ &\le |\psi'(c)| + \|V\psi\|_1 + \left(\int_c^x dt\, |u(t)|^2\right)^{1/2} \left(\int_c^x dt\right)^{1/2} \\ &\le |\psi'(c)| + \|V\psi\|_1 + \|u\|_2 \sqrt{x-c}. \end{aligned}$$

Hence,

$$\begin{aligned} \left|\frac{\psi'(x)}{\sqrt{x}}\right| &\le \frac{|\psi'(c)| + \|V\psi\|_1}{\sqrt{x}} + \frac{\|u\|_2 \sqrt{x-c}}{\sqrt{x}} \\ &\le \frac{|\psi'(c)| + \|V\psi\|_1}{\sqrt{c}} + \|u\|_2 := C, \qquad x > c. \end{aligned}$$

The lemma is proved. □

*Proof.* **[Proposition 7.5.3]** Since 0 is a regular point of $H$ it is in the limit circle case (and $\psi(0), \psi'(0)$ take finite values). So the deficiency indices are equal either to 1 or to 2. It will be checked that $W_\infty[\psi,\varphi] = 0$, $\forall \psi, \varphi \in \operatorname{dom} H^*$, so that $\Gamma_{H^*}(\psi,\varphi) = -W_0[\psi,\varphi] = \varphi(0)\overline{\psi'(0)} - \varphi'(0)\overline{\psi(0)}$ and, as in Example 7.3.1, the self-adjoint extensions of $H$ are parametrized by the complex numbers $e^{i\theta}$; thus the deficiency indices of $H$ are equal to 1. As a subproduct it follows that $H$ is in the limit point case at $\infty$.

Let $\psi \in \operatorname{dom} H^*$; it is known that $W_\infty[\psi,\varphi]$ is finite. Suppose $x > c$; by Lemma 7.5.4,

$$\frac{1}{\sqrt{x}}\, |W_x[\psi,\varphi]| = \left| \overline{\psi(x)} \frac{\psi'(x)}{\sqrt{x}} - \frac{\overline{\psi'(x)}}{\sqrt{x}} \psi(x) \right| \le 2C\, |\psi(x)|\,,$$

so that the right-hand side belongs to $\mathrm{L}^2(c,\infty)$, but the left-hand side does not belong to $\mathrm{L}^2(c,\infty)$ if $W_\infty[\psi,\varphi] \neq 0$. Hence, $W_\infty[\psi,\varphi] = 0$, $\forall \psi \in \operatorname{dom} H^*$. □

*Exercise* 7.5.5. If $V \in \mathrm{L}^2(0,\infty)$, find all self-adjoint extensions of $H$ (see Example 7.3.1).

*Exercise* 7.5.6. Show that if the potential $V \in \mathrm{L}^2_{\mathrm{loc}}(0,\infty)$ is in $\mathrm{L}^2$ near $\infty$, then $\Gamma_{H^*}(\psi,\varphi) = -W_0[\psi,\varphi]$, $\forall \psi,\varphi \in \operatorname{dom} H^*$. Conclude that if $V$ is regular at 0, then the deficiency indices of $H$ are equal to 1.

*Remark* 7.5.7. As discussed in [Win47], for a class of negative potentials $V(x)$, $x \in \mathbb{R}$, satisfying a technical condition and $\lim_{x\to\infty} V(x) = -\infty$, the differential operator $H$ is limit circle at infinity iff, for some $x_0 > 0$, $\int_{x_0}^{\infty} (-V(x))^{-1/2}\, dx < \infty$. In case of $V(x) = -\kappa x^\alpha$, $x > 0$ and $\kappa > 0, \alpha > 0$, $H$ is then limit point at $\infty$ iff $\alpha \le 2$ (this case is included in Wintner's class).

This characterization of limit point at infinity has a counterpart in classical mechanics that is worth mentioning (and appreciating). For a classical particle of mass $m$ and total mechanical energy $E$ under this potential $V(x)$, the travel time from the initial position $x_0 > 0$ to $\infty$ is

$$\tau_\infty = \sqrt{\frac{m}{2}} \int_{x_0}^{\infty} \frac{dx}{\sqrt{E - V(x)}}.$$

This follows from conservation of mechanical energy (check this!). If $x_0 \gg 1$ so that $|V(x)| \gg E$, $\forall x \ge x_0$ (since $\lim_{x\to\infty} V(x) = -\infty$), one has

$$\tau_\infty \approx \sqrt{\frac{m}{2}} \int_{x_0}^{\infty} \frac{dx}{\sqrt{-V(x)}},$$

that is, the condition $\tau_\infty = \infty$ coincides with the limit point criterion, which, in its turn, is a necessary condition for the existence of just one self-adjoint extension of $H$. Hence, for such potentials, a finite travel time to reach infinity in classical mechanics is reflected in the quantum limit circle at infinity, inferring the quantum ambiguity of more than one self-adjoint extension of $H$. However, there are counterexamples to this correspondence between essential self-adjointness and finite travel time to infinity [RaR73].

A discussion, from a physical point of view, of the unitary evolution group generated by $H$ with negative potentials so that $\tau_\infty < \infty$ can be found in [CFGM90].

Additional criteria for limit point and limit circle can be found in [Na69], [ReeS75] and [DuS63]. See also [BaZG04].

### 7.5.1 A Multiply Connected Domain

Some self-adjoint extensions of a hermitian operator with infinite deficiency index will be found. It will combine the spherical symmetry with the topological property of multiply connectedness. Some specific results on Sobolev traces will be invoked; see [Bre99, Ad75] and Chapters 1 and 2 of the first volume of [LiM72]. Nevertheless we think the set of presented results will make this subsection worthwhile; except for Section 10.5, they will not be needed for other parts of the text.

Let $\Lambda = \mathbb{R}^2 \setminus \overline{B}(0;a)$, $a > 0$ (i.e., the plane with a circular hole), and its closure $\overline{\Lambda} = \mathbb{R}^2 \setminus B(0;a)$; its boundary $\partial\Lambda$ is the circumference $S = \{(x_1, x_2) \in$

$\mathbb{R}^2 : r = (x_1^2 + x_2^2)^{\frac{1}{2}} = a\}$. The potential will be a bounded continuous $V : \overline{\Lambda} \to \mathbb{R}$, with $V(x) = V(r)$, and the initial hamiltonian is the hermitian operator

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

What are the self-adjoint extensions of $H$?

As above, polar coordinates $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$ are introduced so that $\mathrm{L}^2(\overline{\Lambda})$ is unitarily equivalent to $\mathrm{L}^2_{rdr}([a,\infty)) \otimes \mathrm{L}^2_{d\varphi}(S)$, and consider the functions $e_m(\varphi) = e^{im\varphi}/\sqrt{2\pi}$, $0 \le \varphi \le 2\pi, m \in \mathbb{Z}$, so that

$$H(Re_m) = \left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2} + V(r)\right) Re_m.$$

After performing the unitary transformation $u_2 : \mathrm{L}^2_{rdr}([a,\infty)) \to \mathrm{L}^2_{dr}([a,\infty))$, $(u_2 R)(r) = \sqrt{r}R(r)$, the operator $u_2 H u_2^{-1}$ restricted to the subspace spanned by $e_m$ takes the form

$$\hat{H}_m = -\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{r^2} + V(r), \qquad \operatorname{dom} \hat{H}_m = C_0^\infty(a,\infty).$$

The original problem is thus reduced to the study of infinitely many Schrödinger operators on $[a,\infty)$ with potentials

$$\hat{V}_m(r) = (m^2 - 1/4)/r^2 + V(r), \qquad m \in \mathbb{Z}.$$

One then easily checks that, for all $m$, the deficiency indices of $H_m$ are equal to 1 (the point here is that $a > 0$, instead of $a = 0$ previously discussed), so that $n_+(H) = \infty = n_-(H)$.

The subject now is to recall Sobolev traces in a convenient way. Although a $\psi(r,\varphi) \in \mathcal{H}^1(\Lambda)$ is not necessarily continuous, it is possible to give a meaning to the restriction $\psi(a,\varphi) = \psi|_{\partial\Lambda}(\varphi) \in \mathrm{L}^2(S)$ via the so-called *Sobolev trace* of $\psi$ (see below), that is, the trace of $\psi$ is interpreted as its value on the boundary of $\Lambda$.

Let $\mathcal{R}C_0^1(\mathbb{R}^2)$ be the restriction of $C_0^1(\mathbb{R}^2)$ to $C_0^1(\overline{\Lambda})$ (see the references for details); it turns out that there is a continuous linear map $\gamma : \mathcal{R}C_0^1(\mathbb{R}^2) \subset \mathcal{H}^1(\Lambda) \to \mathrm{L}^2(S)$, $\gamma(\phi(r,\varphi)) = \phi(a,\varphi)$, that is, there is $C > 0$ so that

$$\|\gamma\phi\|_{\mathrm{L}^2(S)} = \|\phi(a,\varphi)\|_{\mathrm{L}^2(S)} \le C\,\|\mathcal{R}\phi\|_{\mathcal{H}^1(\Lambda)}, \qquad \phi \in C_0^1(\mathbb{R}^2).$$

Note that for $\phi \in C_0^1(\mathbb{R}^2)$ the boundary values $\phi(a,\varphi)$ are well defined for any angular value $\varphi$. By density, this map has a unique continuous extension (keeping the same notation) $\gamma : \mathcal{H}^1(\Lambda) \to \mathrm{L}^2(S)$, called the *Sobolev trace map*, and one defines the trace of $\psi$ as $\psi(a,\varphi) := \gamma(\psi)$ for all $\psi \in \mathcal{H}^1(\Lambda)$. The essential characteristics here are smoothness and compactness of the boundary $\partial\Lambda$ [Bre99]; some important properties of the trace are as follows.

i) For $\psi \in \mathcal{H}^1(\Lambda)$ the trace is not defined in a pointwise manner, only as a function in $\mathrm{L}^2(S)$. General elements of $\mathrm{L}^2(\Lambda)$ do not have a trace defined.

ii) rng $\gamma$ is dense in $\mathrm{L}^2(S)$ and the Green formula

$$\int_\Lambda \frac{\partial\psi(x)}{\partial x_j}\phi(x)\,dx + \int_\Lambda \psi(x)\frac{\partial\phi(x)}{\partial x_j}\,dx = a\int_0^{2\pi} \psi(a,\varphi)\phi(a,\varphi)\,d\varphi$$

holds for all $\psi, \phi \in \mathcal{H}^1(\Lambda)$, $j = 1, 2$.

iii) The kernel of the trace operator is

$$\mathcal{H}_0^1(\Lambda) := \{\psi \in \mathcal{H}^1(\Lambda) : \gamma(\psi) = \psi(a,\varphi) = 0\},$$

which is a Hilbert space that can also be defined as the closure of $C_0^\infty(\Lambda)$ in $\mathcal{H}^1(\Lambda)$.

iv) In a similar way, if $\psi \in \mathcal{H}^2(\Lambda)$ one has a well-defined trace $\gamma(\partial\psi/\partial r)$, which will be denoted by $\partial\psi/\partial r(a,\varphi)$, which stands for the normal derivative with respect to $\partial\Lambda$ (this is used in the adaptation to more general $\Lambda$) and belongs to $\mathrm{L}^2(\partial\Lambda)$.

v) The ranges of both trace maps $\mathcal{H}^2(\Lambda) \ni \psi \mapsto \psi(a,\varphi)$ and $\mathcal{H}^2(\Lambda) \ni \psi \mapsto \partial\psi/\partial r(a,\varphi)$ are dense in $\mathrm{L}^2(S)$, and the Green formula

$$\int_\Lambda \Delta\psi(x)\phi(x)\,dx + \int_\Lambda \nabla\psi(x)\nabla\phi(x)\,dx = a\int_0^{2\pi} \frac{\partial\psi}{\partial r}(a,\varphi)\phi(a,\varphi)\,d\varphi$$

holds for all $\psi, \phi \in \mathcal{H}^2(\Lambda)$.

Now a subtlety must be mentioned. At first sight one could (wrongly) guess that the domain of the adjoint $H^*$ is $\mathcal{H}^2(\Lambda)$. However, for open sets $\Omega \subset \mathbb{R}^n$, $\Omega \neq \mathbb{R}^n$ and $n \geq 2$, there are functions $\psi \in \mathrm{L}^2(\Omega)$ with distributional laplacian $\Delta\psi \in \mathrm{L}^2(\Omega)$ that do not belong to $\mathcal{H}^2(\Omega)$; the point is that other derivatives, as first derivatives, of $\psi$ need not exist as functions! It turns out that

$$\mathrm{dom}\ H^* = \left\{\psi \in \mathrm{L}^2(\Lambda) : (-\Delta\psi + V\psi) \in \mathrm{L}^2(\Lambda)\right\}$$

and $H^*\psi = -\Delta\psi + V\psi$, $\psi \in \mathrm{dom}\ H^*$, and this domain is strictly larger than $\mathcal{H}^2(\Lambda)$. See [Gru06], [Gru08] and references therein.

By using the above characterization of $H^*$, some self-adjoint extensions of $H$ will be found via suitable restrictions of $H^*$. The boundary form of $H$, for $\psi, \phi \in \mathrm{dom}\ H^*$, is

$$\Gamma(\psi,\phi) := \langle(-\Delta + V)\psi, \phi\rangle - \langle\psi, (-\Delta + V)\phi\rangle.$$

By restricting to those self-adjoint extensions whose domains are contained in $\mathcal{H}^2(\Lambda)$, Sobolev traces can be invoked, the continuity of the potential guarantees that $V|_{\partial\Lambda} = V(a)$ is well posed and the above Green formula can be used to compute, for $\psi, \phi \in \mathcal{H}^2(\Lambda)$,

$$\Gamma(\psi,\phi) = a\int_0^{2\pi} \left(\overline{\psi(a,\varphi)}\,\frac{\partial\phi}{\partial r}(a,\varphi) - \overline{\frac{\partial\psi}{\partial r}(a,\varphi)}\,\phi(a,\varphi)\right)\,d\varphi.$$

Introduce $\rho_j : \mathcal{H}^2(\Lambda) \to \mathrm{L}^2(S)$, $j = 1, 2$, by

$$\rho_1(\psi) = \psi(a,\varphi) + i\frac{\partial\psi}{\partial r}(a,\varphi),$$
$$\rho_2(\psi) = \psi(a,\varphi) - i\frac{\partial\psi}{\partial r}(a,\varphi),$$

and so

$$(2i/a)\,\Gamma(\psi,\phi) = \langle\rho_1(\psi),\rho_1(\phi)\rangle_{\mathrm{L}^2(S)} - \langle\rho_2(\psi),\rho_2(\phi)\rangle_{\mathrm{L}^2(S)}\,.$$

*Exercise* 7.5.8. Verify the above two expressions for the boundary form $\Gamma(\psi,\phi)$ of $H$, for $\psi,\phi \in \mathcal{H}^2(\Lambda)$.

A boundary triple for $H$ in the Sobolev space $\mathcal{H}^2(\Lambda)$ has been found with $\mathbf{h} = \mathrm{L}^2(S)$. As before (i.e., by Theorem 7.1.13), from this boundary triple the self-adjoint extensions $H_U$ of $H$ in $\mathcal{H}^2(\Lambda)$ are characterized by unitary operators $U : \mathrm{L}^2(S) \hookleftarrow$ so that $\rho_1(\psi) = U\rho_2(\psi)$, $\forall\psi \in \mathrm{dom}\; H_U$, and $H_U\psi = H^*\psi$. After writing out this relation one finds

$$(\mathbf{1} - U)\,\psi(a,\varphi) = -i(\mathbf{1} + U)\frac{\partial\psi}{\partial r}(a,\varphi).$$

Therefore, all self-adjoint extensions of $H$ with domain in $\mathcal{H}^2(\Lambda)$ were found and they are realized through suitable boundary conditions on $\partial\Lambda$; such boundary conditions are in terms of traces of elements of $\mathcal{H}^2(\Lambda)$. Below some explicit self-adjoint extensions are described.

1. $U = -\mathbf{1}$.

   In this case

   $$\mathrm{dom}\; H_U = \{\psi \in \mathcal{H}^2(\Lambda) : \psi(a,\varphi) = 0\} = \mathcal{H}^2(\Lambda) \cap \mathcal{H}^1_0(\Lambda),$$

   $H_U\psi = (-\Delta + V)\psi$, $\psi \in \mathrm{dom}\; H_U$. This is the so-called Dirichlet realization (of the laplacian if $V = 0$) in $\Lambda$.

2. $U = \mathbf{1}$.

   In this case $\mathrm{dom}\; H_U = \{\psi \in \mathcal{H}^2(\Lambda) : \partial\psi/\partial r(a,\varphi) = 0\}$, $H_U\psi = (-\Delta + V)\psi$. This is the so-called Neumann realization.

3. $(\mathbf{1} + U)$ is invertible.

   In this case one gets that for each self-adjoint operator $A : \mathrm{dom}\; A \sqsubseteq \mathrm{L}^2(S) \to \mathrm{L}^2(S)$ corresponds a self-adjoint extension $H^A$. In fact, first pick a unitary operator $U_A$ so that $A = -i(\mathbf{1} - U_A)(\mathbf{1} + U_A)^{-1}$, $\mathrm{dom}\; A = \mathrm{rng}\;(\mathbf{1}+U_A)$ and $\mathrm{rng}\; A = \mathrm{rng}\;(\mathbf{1}-U_A)$; recall the Cayley transform in Chapter 2. Now, $\mathrm{dom}\; H^A$ is the set of $\psi \in \mathcal{H}^2(\Lambda)$ with "$\partial\psi/\partial r(a,\cdot) = A\psi(a,\cdot)$," prudently understood in the sense that

   $$(\mathbf{1} - U_A)\,\psi(a,\varphi) = -i(\mathbf{1} + U_A)\frac{\partial\psi}{\partial r}(a,\varphi),$$

   in order to avoid domain questions. Of course the quotation marks can be removed in case the operator $A$ is bounded.

Similarly, for each self-adjoint $B$ acting in $L^2(S)$ there corresponds a unitary $U_B$, and if $(\mathbf{1} - U_B)$ is invertible, then there corresponds the self-adjoint extension $H^B$ of $H$ with dom $H^B$ the set of $\psi \in \mathcal{H}^2(\Lambda)$ so that "$\psi(a, \cdot) = B\frac{\partial \psi}{\partial r} r(a, \cdot)$," in the sense that

$$(\mathbf{1} - U_B)\,\psi(a, \varphi) = -i(\mathbf{1} + U_B)\frac{\partial \psi}{\partial r}(a, \varphi).$$

Again the quotation marks can be removed in case the operator $B$ is bounded.

Note that 4 below is, in fact, particular cases of 3 in which $A = \mathcal{M}_f$ and $B = \mathcal{M}_g$.

4. $U$ is a multiplication operator.

Given a real-valued (measurable) function $u(\varphi)$ put $U = \mathcal{M}_{e^{iu(\varphi)}}$. If $\{\varphi : \exp(iu(\varphi)) = -1\}$ has measure zero, then

$$f(\varphi) = -i\frac{1 - e^{iu(\varphi)}}{1 + e^{iu(\varphi)}}$$

is (measurable) well defined and real valued. The domain of the corresponding self-adjoint extension is

$$\text{dom } H_U = \left\{\psi \in \mathcal{H}^2(\Lambda) : \partial\psi/\partial r(a, \varphi) = f(\varphi)\psi(a, \varphi)\right\}.$$

Similarly, if $\{\varphi : \exp(iu(\varphi)) = 1\}$ has measure zero,

$$g(\varphi) = i\frac{1 + e^{iu(\varphi)}}{1 - e^{iu(\varphi)}}$$

is real valued and the domain of the subsequent self-adjoint extension is

$$\text{dom } H_U = \{\psi \in \mathcal{H}^2(\Lambda) : \psi(a, \varphi) = g(\varphi)\partial\psi/\partial r(a, \varphi)\}.$$

Special cases are given by constant functions $f, g$.

5. $A = -id/d\varphi$ with domain $\mathcal{H}^1(S) = \{u \in \mathcal{H}^1(0, 2\pi) : u(0) = u(2\pi)\}$. The corresponding self-adjoint extension has domain

$$\left\{\psi \in \mathcal{H}^2(\Lambda) : \psi(a, \varphi) \in \mathcal{H}^1(S), \text{``}\frac{\partial \psi}{\partial r}(a, \varphi) = -i\frac{d\psi}{d\varphi}(a, \varphi)\text{''}\right\}.$$

*Exercise* 7.5.9. Show that $A = -id/d\varphi$ in 5 above is self-adjoint.

Since the deficiency indices of $H$ are infinite, there is a plethora of self-adjoint extensions of the laplacian in the multiply connected domain $\Lambda = \mathbb{R}^2 \setminus \overline{B}(0; a)$. Some of them can be quite unusual and hard to understand from the physical and mathematical points of view.

*Remark* 7.5.10. The choice of $\Lambda = \mathbb{R}^2 \setminus \overline{B}(0;a)$ was for notational convenience. In a similar way one finds expressions for the boundary form of $H = -\Delta + V$ with domain $C_0^\infty(\mathbb{R}^2 \setminus \overline{\Omega})$, with $\Omega \subset \mathbb{R}^2$ an open set with compact boundary $\partial\Omega$ of class $C^1$; when restricted to domains in $\mathcal{H}^2(\mathbb{R}^2 \setminus \Omega)$, Sobolev traces are properly defined in this setting, and one can also consider $\mathbb{R}^n$, $n \geq 2$. For such more general multiply connected regions, one must consider the normal derivative $\partial\psi/\partial\mathbf{n}$ at the boundary $\partial\Omega$, instead of $\partial\psi/\partial r$, and also the corresponding modifications in the expressions of Green formulae [Bre99], [LiM72].

*Remark* 7.5.11. The above approach to the self-adjoint extensions of the laplacian in $\mathcal{H}^2(\Lambda)$ was borrowed from [deO08], as well as the variation of the concept of boundary triple. However, by using a continuous extension of the trace maps to the dual Sobolev spaces $\mathcal{H}^{-1/2}(\partial\Lambda)$ and $\mathcal{H}^{-3/2}(\partial\Lambda)$, in [Gru06] one finds references and comments to her previous works on all self-adjoint extensions of the laplacian in terms of self-adjoint operators from closed subspaces of $\mathcal{H}^{-1/2}(\partial\Lambda)$.

*Exercise* 7.5.12. Let $0 < a < b < \infty$ and

$$\Lambda_{ab} = \left\{(x_1, x_2) \in \mathbb{R}^2 : a < (x_1^2 + x_2^2)^{\frac{1}{2}} < b\right\}$$

be an annulus in $\mathbb{R}^2$. Find the self-adjoint extensions of the laplacian $H_0 = -\Delta$, dom $H_0 = C_0^\infty(\Lambda_{ab})$, whose domains are contained in $\mathcal{H}^2(\Lambda_{ab})$.