Chapter 4

Operators via Sesquilinear Forms

The basics of self-adjoint extensions via sesquilinear forms are discussed. The main points are form representations, Friedrichs extensions and examples. Additional information appears in Sections 6.1, 9.3 and 10.4. Some sesquilinear forms can be sources of self-adjoint operators related to "singular interactions" and/or ill-posed operator sums.

4.1 Sesquilinear Forms

Let dom b be a dense subspace of the Hilbert space $\mathcal{H}$. A *sesquilinear form* in $\mathcal{H}$,

$$b : \mathrm{dom}\ b \times \mathrm{dom}\ b \to \mathbb{C}$$

is a map linear in the second variable and antilinear in the first one. b is hermitian if $b(\xi, \eta) = \overline{b(\eta, \xi)}$. The map $\xi \mapsto b(\xi, \xi)$, $\xi \in \mathrm{dom}\ b$, is called the *quadratic form* associated with b. Usually dom b is referred to as the domain of b, instead of dom $b \times$ dom b, and only the term *form* is used as a shorthand for sesquilinear form. Sometimes the notation $b(\xi) = b(\xi, \xi)$ for the quadratic form is used. Here all forms are assumed to be densely defined.

Exercise 4.1.1. Verify the polarization identity for sesquilinear forms

$$4b(\xi, \eta) = b(\xi + \eta) - b(\xi - \eta) - ib(\xi + i\eta) + ib(\xi - i\eta),$$

for all $\xi, \eta \in \mathrm{dom}\ b$. Use polarization to show that b is hermitian iff the associated quadratic form is real valued.

Definition 4.1.2. A sesquilinear form b is *bounded* if its *form norm*

$$\|b\| := \sup_{\substack{0\neq\xi_1\in\mathrm{dom}\ b\\ 0\neq\xi_2\in\mathrm{dom}\ b}} \frac{|b(\xi_1,\xi_2)|}{\|\xi_1\|\,\|\xi_2\|}$$

is finite, i.e., $\|b\| < \infty$.

The standard example of bounded sesquilinear form is the inner product on a Hilbert space, whose norm is 1. The next result is the structure of bounded sesquilinear forms; the corresponding results when boundedness is not required appear in Theorems 4.2.6 and 4.2.9.

Proposition 4.1.3. *If $b : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ is a bounded sesquilinear form, then there exists a unique operator $T_b \in \mathrm{B}(\mathcal{H})$ obeying*

$$b(\xi_1, \xi_2) = \langle T_b\xi_1, \xi_2\rangle, \qquad \forall \xi_1, \xi_2 \in \mathcal{H}.$$

Furthermore, $\|T_b\| = \|b\|$ and if b is hermitian then T_b is self-adjoint.

Proof. For each $\xi_1 \in \mathcal{H}$ the functional $L_{\xi_1} : \mathcal{H} \to \mathbb{C}$, $L_{\xi_1}(\xi_2) = b(\xi_1, \xi_2)$ is linear, and since

$$|L_{\xi_1}(\xi_2)| = |b(\xi_1, \xi_2)| \leq \|b\|\|\xi_1\|\,\|\xi_2\|,$$

then $\|L_{\xi_1}\| \leq \|b\|\,\|\xi_1\|$ and $L_{\xi_1} \in \mathcal{H}^*$ (the dual space of $\mathcal{H}$).

By Riesz's Representation Theorem 1.1.40 there exists a unique $\eta_2 \in \mathcal{H}$ with $L_{\xi_1}(\xi_2) = \langle \eta_2, \xi_2\rangle$, for all $\xi_2 \in \mathcal{H}$. Define $T_b : \mathcal{H} \to \mathcal{H}$ by $T_b\xi_1 = \eta_2$, for which $b(\xi_1, \xi_2) = \langle T_b\xi_1, \xi_2\rangle$, $\forall \xi_1 \in \mathcal{H}, \xi_2 \in \mathcal{H}$, and it is linear. Note that $T_b = 0$ if, and only if, b is null (the definition is clear!).

Thus, if $b \neq 0$,

$$\begin{aligned}\|T_b\| &= \sup_{\substack{0\neq\xi_1\\ T_b\xi_1\neq 0}} \frac{\|T_b\xi_1\|}{\|\xi_1\|} = \sup_{\substack{0\neq\xi_1\\ T_b\xi_1\neq 0}} \frac{|\langle T_b\xi_1, T_b\xi_1\rangle|}{\|\xi_1\|\,\|T_b\xi_1\|} \leq \|b\| \\ &= \sup_{\substack{0\neq\xi_1\\ 0\neq\xi_2}} \frac{|\langle T_b\xi_1, \xi_2\rangle|}{\|\xi_1\|\,\|\xi_2\|} \leq \sup_{\substack{0\neq\xi_1\\ 0\neq\xi_2}} \frac{\|T_b\xi_1\|\,\|\xi_2\|}{\|\xi_1\|\,\|\xi_2\|} = \|T_b\|,\end{aligned}$$

showing that $T_b \in \mathrm{B}(\mathcal{H})$ and $\|T_b\| = \|b\|$. The uniqueness of the operator follows from the relation $\langle T_b\xi_1, \xi_2\rangle = \langle S\xi_1, \xi_2\rangle$, for any ξ_1, ξ_2, consequently the operators S and T_b coincide.

Now if such b is hermitian then $\langle T_b\xi, \eta\rangle = b(\xi, \eta) = \overline{b(\eta, \xi)} = \langle \xi, T_b\eta\rangle$, and T_b is self-adjoint. □

Hence, there is a one-to-one correspondence between such bounded (and hermitian) sesquilinear forms on $\mathcal{H} \times \mathcal{H}$ and bounded (and self-adjoint) linear operators on $\mathcal{H}$. Observe that if the sesquilinear form is given by the inner product on $\mathcal{H}$, then Proposition 4.1.3 gives rise to the identity operator $T_b = \mathbf{1}$.

One then wonders whether it is possible to adapt the above construction to get unbounded self-adjoint operators from more general forms. In fact, part of this construction can be carried out for suitable forms, as discussed below; a chief result will be that there is a one-to-one correspondence between "closed lower bounded sesquilinear forms" and lower bounded self-adjoint operators. Other motivations appear in Remark 4.1.14. Now some definitions.

Definition 4.1.4. Let b be a hermitian sesquilinear form. Then b is:

a) *positive* if the quadratic form $b(\xi,\xi) \geq 0, \forall \xi \in \text{dom } b$.
b) *lower bounded* if there is $\beta \in \mathbb{R}$ with $b(\xi,\xi) \geq \beta \|\xi\|^2$, $\forall \xi \in \text{dom } b$, and this situation will be briefly denoted by $b \geq \beta$; such β is called a *lower limit* or *lower bound* of b. Notice that $b - \beta$ defines a positive sesquilinear form by $(b-\beta)(\xi,\eta) := b(\xi,\eta) - \beta\langle \xi,\eta\rangle$.

Exercise 4.1.5. Verify that Cauchy-Schwarz and triangular inequalities

$$|b(\xi,\eta)| \leq b(\xi)^{\frac{1}{2}}\, b(\eta)^{\frac{1}{2}}, \qquad b(\xi+\eta)^{\frac{1}{2}} \leq b(\xi)^{\frac{1}{2}} + b(\eta)^{\frac{1}{2}},$$

respectively, hold for positive sesquilinear forms ($\forall \xi,\eta \in \text{dom } b$).

Let b be a hermitian form and $(\xi_n) \subset \text{dom } b$. Even though b is not necessarily positive, this sequence is called a *Cauchy sequence* with respect to b (or in $(\text{dom } b, b)$) if $b(\xi_n - \xi_m) \to 0$ as $n,m \to \infty$. It is said that (ξ_n) *converges* to ξ with respect to b (or in $(\text{dom } b, b)$) if $\xi \in \text{dom } b$ and $b(\xi_n - \xi) \to 0$ as $n \to \infty$.

Definition 4.1.6. A sesquilinear form b is *closed* if for each Cauchy sequence (ξ_n) in $(\text{dom } b, b)$ with $\xi_n \to \xi$ in $\mathcal{H}$, one has $\xi \in \text{dom } b$ and $\xi_n \to \xi$ in $(\text{dom } b, b)$. b is *closable* if it has a closed extension in $\mathcal{H}$.

If β is a lower bound of the sesquilinear form b, one introduces the inner product $\langle \cdot,\cdot\rangle_+$ on $\text{dom } b \subset \mathcal{H}$ by the expression

$$\langle \xi,\eta\rangle_+ := b(\xi,\eta) + (1-\beta)\langle \xi,\eta\rangle,$$

and one has $\langle \xi,\xi\rangle_+ = b(\xi,\xi) - \beta\|\xi\|^2 + \|\xi\|^2 \geq \|\xi\|^2$, so that the norm $\|\xi\|_+ := \sqrt{\langle \xi,\xi\rangle_+} \geq \|\xi\|$.

Definition 4.1.7.

a) If $b \geq \beta$, the abstract completion of the inner product space $(\text{dom } b, \langle \cdot,\cdot\rangle_+)$ will be denoted by $(\mathcal{H}_+, b_+)$.
b) Let b denote a closed and lower bounded form $b \geq \beta$. A *form core* of b is a subset $\mathcal{D} \subset \text{dom } b$ which is dense in $\text{dom } b$ equipped with the inner product $\langle \cdot,\cdot\rangle_+ = b_+(\cdot)$.

Remark 4.1.8. If $b \geq \beta \geq 0$ is closed and also an inner product, then $\mathcal{D}$ is a form core of b is equivalent to $\mathcal{D}$ being dense in $(\text{dom } b, b)$, i.e., it is not necessary to take $\langle \cdot,\cdot\rangle_+$. This applies, in particular, when a form core of $\langle \cdot,\cdot\rangle_+$ is considered.

Lemma 4.1.9. *Suppose that the hermitian sesquilinear form $b \geq \beta$, for some $\beta \in \mathbb{R}$. Then the following assertions are equivalent:*

i) $(\mathrm{dom}\ b, \langle\cdot,\cdot\rangle_+)$ *is a Hilbert space* (*and so it coincides with* $(\mathcal{H}_+, b_+)$).
ii) b *is closed.*

Proof. First note that every Cauchy sequence in $\mathcal{K} := (\mathrm{dom}\ b, \langle\cdot,\cdot\rangle_+)$ is also a Cauchy sequence in the other three spaces: $\mathcal{H}$, $(\mathrm{dom}\ b, b-\beta)$ and also in $(\mathrm{dom}\ b, b)$.

Suppose that i) holds. If (ξ_n) is Cauchy in $\mathcal{K}$ then there is $\xi \in \mathrm{dom}\ b$ so that $\xi_n \to \xi$ in $\mathcal{K}$; also $\|\xi_n - \xi\| \to 0$ and so $\xi_n \to \xi$ in $\mathcal{H}$. That is, ii) holds.

Conversely, suppose that ii) holds. If (ξ_n) is Cauchy in $\mathcal{K}$, then it is also Cauchy with respect to b and in $\mathcal{H}$, and so there is ξ with $\xi_n \to \xi$ in $\mathcal{H}$. By ii), $\xi \in \mathrm{dom}\ b$ and $\xi_n \to \xi$ in $\mathcal{K}$. So $\mathcal{K}$ is complete, that is, i) holds. □

The above lemma shows that any lower bound β can be used to construct $\mathcal{H}_+$; in particular if $b \geq \beta > 0$, a preferred choice is the zero lower bound. Note that $b_+(\cdot,\cdot)$ is the inner product on the Hilbert space $\mathcal{H}_+$ and if $\xi, \eta \in \mathrm{dom}\ b$, then $b_+(\xi,\eta) = \langle\xi,\eta\rangle_+$; moreover, b_+ is a closed sesquilinear form on $\mathcal{H}_+$.

Example 4.1.10. To a densely defined operator T one introduces two positive hermitian sesquilinear forms $b, \tilde{b}$, with $\mathrm{dom}\ b = \mathrm{dom}\ \tilde{b} = \mathrm{dom}\ T$, via $b(\xi,\eta) = \langle T\xi, T\eta\rangle$ and $\tilde{b}(\xi,\eta) = \langle T\xi, T\eta\rangle + \langle\xi,\eta\rangle$. Since $\tilde{b}(\xi,\xi) = \|\xi\|_T^2$, i.e., the square of the graph norm of T, it is closed iff T is closed; one has $\tilde{b} \geq 1$. See also Example 4.1.11.

Note that $\tilde{b}(\xi,\eta) = b(\xi,\eta) + \langle\xi,\eta\rangle$; this was a motivation for the introduction of the inner product $\langle\xi,\eta\rangle_+$ and the definition of closed form above.

Example 4.1.11. A hermitian operator $T : \mathrm{dom}\ T \sqsubseteq \mathcal{H} \to \mathcal{H}$ defines a hermitian sesquilinear form b^T as

$$b^T(\xi,\eta) := \langle\xi, T\eta\rangle, \qquad \mathrm{dom}\ b^T = \mathrm{dom}\ T.$$

b^T is lower bounded iff T is (see Definition 2.4.16). Since this b^T is easily extended to any $\xi \in \mathcal{H}$ and $\eta \in \mathrm{dom}\ T$, it has a potential advantage over the forms in Example 4.1.10 while searching extensions of T. See Theorem 4.3.1.

Definition 4.1.12. If $T : \mathrm{dom}\ T \sqsubseteq \mathcal{H} \to \mathcal{H}$ is a hermitian operator, the form b^T introduced in Example 4.1.11 is called the sesquilinear form *generated by* T.

Remark 4.1.13. In the specific case of positive self-adjoint operators $T \geq 0$, the form b^T generated by T will be naturally extended in Section 9.3, and keeping the same notation b^T and nomenclature, to the form $\mathrm{dom}\ b^T = \mathrm{dom}\ T^{\frac{1}{2}}$, $b^T(\xi,\eta) = \langle T^{\frac{1}{2}}\xi, T^{\frac{1}{2}}\eta\rangle$, $\forall \xi,\eta \in \mathrm{dom}\ T^{\frac{1}{2}}$. Refer to Section 9.3 for explanation of these symbols.

Remark 4.1.14. There are many appealing reasons for considering sesquilinear forms as sources of operators.

- In physics it is a common procedure to deal with "matrix elements" of an operator, i.e., $b^T(\xi,\eta) = \langle\xi, T\eta\rangle$. Also $\langle\xi, T\xi\rangle$ is the expectation value of the observable T (see discussion on page 132) if the system is in the normalized state ξ, and one asks how to construct the (self-adjoint) operator T from its matrix elements. Some authors argue that physically the expectation values are more fundamental than the square $\|T\xi\|^2 = \langle T\xi, T\xi\rangle$.

- Usually the conditions on the form domain are less restrictive than the ones on the operator domain. For instance, for the second derivative operator $\psi \mapsto -\psi''$, in suitable subspaces of $L^2(\mathbb{R})$, on integrating by parts one can write $\langle \psi, -\phi''\rangle = \langle \psi', \phi'\rangle$, and the right-hand side inner product imposes conditions only on the first derivative of the functions.
- Given hermitian operators T_1, T_2 and a form b, due to less stringent domain conditions (e.g., $\mathrm{dom}\ T_1 \cap \mathrm{dom}\ T_2$ can be rather small), sesquilinear forms open the possibility of defining an operator T via the sum of forms by imposing $b^T(\xi,\eta) = b^{T_1}(\xi,\eta) + b^{T_2}(\xi,\eta)$ (see Example 4.2.15, Corollary 9.3.12 and Subsection 9.3.1), and also through $b^T(\xi,\eta) = b^{T_1}(\xi,\eta) + b(\xi,\eta)$ even in some cases b is not directly related to an operator; see Examples 4.1.15, 4.4.9, 6.2.16 and 6.2.19.

The primary point relates to the representation theorems in Section 4.2, which associate self-adjoint operators to forms. Eventually, other reasons supporting the use of sesquilinear forms will appear spread over the book.

Example 4.1.15. Let $\mathrm{dom}\ b_\delta = \mathcal{H}^1(\mathbb{R}) \subset \mathcal{H} = L^2(\mathbb{R})$, and the action

$$b_\delta(\psi, \phi) = \overline{\psi(0)}\, \phi(0), \qquad \psi, \phi \in \mathrm{dom}\ b_\delta.$$

This form is hermitian and positive, but not closable. In fact, the sequence $\psi_n(x) = e^{-nx^2}$ is contained in $\mathrm{dom}\ b_\delta$, $b_\delta(\psi_n - \psi_m) \to 0$ (so a Cauchy sequence with respect to b_δ) and converges to zero in $\mathcal{H}$, but $b_\delta(\psi_n) \to 1$ while $b_\delta(0,0) = 0$ (apply Lemma 4.1.9). Thus, in contrast to hermitian operators, a (lower bounded) hermitian form need not be closable.

Nevertheless, by naively pushing on the comparison with b^T, one would get

$$\overline{\psi(0)}\phi(0) = \langle \psi, T\phi\rangle = \int_{\mathbb{R}} \overline{\psi(x)}T\phi(x)\, dx,$$

and this form should represent an operator T "generated by the Dirac delta $\delta(x)$ at the origin;" such informal association can be useful in some contexts, as in Examples 4.4.9 and 6.2.16 in attempts to make sense of a Schrödinger operator with a delta potential. Clearly $\mathcal{H}^1(\mathbb{R})$ can be replaced by other domains, e.g., $C_0^\infty(\mathbb{R})$.

Remark 4.1.16. Sometimes it is convenient to put $b(\xi,\xi) = \infty$ if $\xi \in \mathcal{H} \setminus \mathrm{dom}\ b$. See Theorem 9.3.11 and Subsection 10.4.1.

4.2 Operators Associated with Forms

Definition 4.2.1. Consider the lower bounded sesquilinear form $b \geq \beta$. b_+ as above is *compatible with* $\mathcal{H}$ if $\mathcal{H}_+$ can be identified with a vector subspace of $\mathcal{H}$ and the (linear) inclusion $j : \mathcal{H}_+ \to \mathcal{H}$ is continuous.

Lemma 4.2.2. *If b_+ is compatible with $\mathcal{H}$, then the inclusion $j : \mathcal{H}_+ \to \mathcal{H}$ can be taken as the natural inclusion $j(\xi) = \xi$, $\forall \xi \in \mathcal{H}_+$, with $\|j\| \leq 1$.*

Proof. The natural inclusion $\hat{j} : (\mathrm{dom}\ b, \langle \cdot, \cdot \rangle_+) \to \mathcal{H}$, $\hat{j}(\xi) = \xi$, is linear and satisfies

$$\|\xi\|^2 = \|\hat{j}(\xi)\|^2 \leq \langle \xi, \xi \rangle_+ = b_+(\xi, \xi),$$

and so it is continuous with $\|\hat{j}\| \leq 1$. Since b_+ is compatible with $\mathcal{H}$, $\hat{j}$ has a unique linear extension $j : \mathcal{H}_+ \to \mathcal{H}$, with $\|j\| \leq 1$.

If $\xi \in \mathcal{H}_+$, there is a sequence $(\xi_k) \subset \mathrm{dom}\ b$ with $\xi_k \to \xi$ in $\mathcal{H}_+$; the above inequality implies $\xi_k \to \xi$ in $\mathcal{H}$. Thus,

$$\begin{aligned} 0 &= \lim_{k\to\infty} j(\xi_k - \xi) = \lim_{k\to\infty} j(\xi_k) - j(\xi) \\ &= \lim_{k\to\infty} \xi_k - j(\xi) = \xi - j(\xi). \end{aligned}$$

Therefore $j(\xi) = \xi$ and j is clearly injective. □

Exercise 4.2.3. Let $(\mathcal{H}_+^{b_\delta}, b_{\delta+})$ be the abstract completion of $(\mathrm{dom}\ b_\delta, b_\delta + 1)$, b_δ the form in Example 4.1.15. Show that the extension j of the natural inclusion $\hat{j} : (\mathrm{dom}\ b_\delta, \langle \cdot, \cdot \rangle_+) \to \mathcal{H}$, $\hat{j}(\xi) = \xi$, $\forall \xi \in \mathrm{dom}\ b_\delta$, is not injective. Conclude that $b_{\delta+}$ is not compatible with $\mathcal{H}$.

Example 4.2.4. Let $T : \mathrm{dom}\ T \sqsubseteq \mathcal{H} \to \mathcal{H}$ be a hermitian and lower bounded operator with lower bound $\beta \in \mathbb{R}$, that is, $T \geq \beta\mathbf{1}$. Consider the form b^T generated by T, the inner product

$$\begin{aligned} \langle \xi, \eta \rangle_+ &= b^T(\xi, \eta) + (1 - \beta)\langle \xi, \eta \rangle \\ &= \langle \xi, (T - \beta\mathbf{1})\eta \rangle + \langle \xi, \eta \rangle, \qquad \xi, \eta \in \mathrm{dom}\ T, \end{aligned}$$

and its completion $(\mathcal{H}_+^T, b_+^T)$. The subject now is to show that b_+^T is compatible with $\mathcal{H}$; consequently b^T is closable.

The linear natural inclusion $\hat{j} : (\mathrm{dom}\ T, \langle \cdot, \cdot \rangle_+) \to \mathcal{H}$, $\hat{j}(\xi) = \xi$, satisfies

$$\|\hat{j}(\xi)\|^2 = \|\xi\|^2 \leq \|\xi\|^2 + \langle \xi, (T - \beta\mathbf{1})\xi \rangle = \langle \xi, \xi \rangle_+,$$

and so it is continuous with $\|\hat{j}\| \leq 1$. Thus $\hat{j}$ has a unique linear extension $j : \mathcal{H}_+^T \to \mathcal{H}$ and with $\|j\| \leq 1$. If $j(\xi) = 0$, then there exists a sequence $(\xi_k) \subset (\mathrm{dom}\ T, \langle \cdot, \cdot \rangle_+)$ with $\xi_k \to \xi$ in $\mathcal{H}_+^T$ and $\xi_k = j(\xi_k) \to 0$ in $\mathcal{H}$. Thus, for any $\eta \in \mathrm{dom}\ T$,

$$\begin{aligned} b_+^T(\eta, \xi) &= \lim_{k\to\infty} b_+^T(\eta, j(\xi_k)) = \lim_{k\to\infty} b_+^T(\eta, \xi_k) \\ &= \lim_{k\to\infty} \langle \eta, \xi_k \rangle_+ = \lim_{k\to\infty} \left(\langle \eta, (T - \beta\mathbf{1})\xi_k \rangle + \langle \eta, \xi_k \rangle\right) \\ &= \lim_{k\to\infty} \langle [T + (1 - \beta)\mathbf{1}]\eta, \xi_k \rangle = 0. \end{aligned}$$

Since dom $T \sqsubseteq \mathcal{H}_+^T$, it follows that $\xi = 0$. Therefore, besides $\|j\| \le 1$, it was found that j is injective and so it is possible to regard $\mathcal{H}_+^T$ as a vector subspace of $\mathcal{H}$, that is, b_+^T is compatible with $\mathcal{H}$. Finally, by Lemma 4.2.2, $j(\xi) = \xi$ for all $\xi \in \mathcal{H}_+^T$.

Given a densely defined operator T, the sesquilinear form $\tilde{b}$ with dom $\tilde{b}$ = dom T, $\tilde{b}(\xi, \eta) := \langle \eta, \xi \rangle_T = \langle T\eta, T\xi \rangle + \langle \eta, \xi \rangle$, satisfies $\tilde{b}(\xi, \xi) \ge \|\xi\|^2$, $\forall \xi \in$ dom $\tilde{b}$, and it is closed iff T is closed. Now if $\eta \in$ dom (T^*T), then

$$\tilde{b}(\xi, \eta) = \langle \xi, (T^*T + \mathbf{1})\eta \rangle, \qquad \forall \xi \in \text{dom } \tilde{b},$$

and, on the basis of Example 4.1.11 and Proposition 4.1.3, one is tempted to link the operator $T^*T + \mathbf{1}$ to $\tilde{b}$. With this motivation in mind, one has the main theorem of this section, ensuring that closed lower bounded forms are actually the forms of lower bounded self-adjoint operators.

Definition 4.2.5. Given a hermitian sesquilinear form b, the *operator* T_b *associated with* b is defined as

$$\begin{aligned} \text{dom } T_b &:= \{\xi \in \text{dom } b : \exists \zeta \in \mathcal{H} \text{ with } b(\eta, \xi) = \langle \eta, \zeta \rangle, \ \forall \eta \in \text{dom } b\}, \\ T_b \xi &:= \zeta, \qquad \xi \in \text{dom } T_b, \end{aligned}$$

that is, $b(\eta, \xi) = \langle \eta, T_b \xi \rangle$, $\forall \eta \in$ dom b, $\forall \xi \in$ dom T_b. Such operator T_b is well defined since dom b is dense in $\mathcal{H}$.

Note that T_b is automatically symmetric; for $\xi, \eta \in$ dom T_b,

$$\langle \eta, T_b \xi \rangle = b(\eta, \xi) = \overline{b(\xi, \eta)} = \overline{\langle \xi, T_b \eta \rangle} = \langle T_b \eta, \xi \rangle.$$

Furthermore, in case of a bounded hermitian sesquilinear form b, the operator T_b in Definition 4.2.5 coincides with the one in Proposition 4.1.3.

The next two theorems are known as representations of sesquilinear forms.

Theorem 4.2.6. *Let* dom $b \sqsubseteq \mathcal{H}$ *and* $b :$ dom $b \times$ dom $b \to \mathbb{C}$ *be a closed sesquilinear form with lower bound* $\beta \in \mathbb{R}$ *(so hermitian).*

Then the operator T_b *associated with* b *is the unique self-adjoint operator with* dom $T_b \sqsubseteq$ dom $b \mapsto \mathcal{H}$ *so that*

$$b(\eta, \xi) = \langle \eta, T_b \xi \rangle, \qquad \forall \eta \in \text{dom } b, \ \forall \xi \in \text{dom } T_b.$$

Further, $T_b \ge \beta\mathbf{1}$ *and* dom T_b *is a form core of* b*. The subspace* dom b *is called the form domain of* T_b*.*

Proof. Set $\mathcal{H}_b :=$ (dom $b, \langle \cdot, \cdot \rangle_+$), which is a Hilbert space by hypothesis. As remarked above, T_b is symmetric. For $\xi \in$ dom $T_b \subset$ dom b one has

$$\langle \xi, T_b \xi \rangle = b(\xi, \xi) \ge \beta \|\xi\|^2,$$

so that $T_b \ge \beta\mathbf{1}$.

For all $\eta \in \mathcal{H}_b$ one has $\|\eta\|_+^2 = \langle \eta, \eta\rangle_+ = (b(\eta) - \beta\|\eta\|^2) + \|\eta\|^2\| \geq \|\eta\|^2$; thus, for each $\phi \in \mathcal{H}$,

$$|\langle \phi, \eta\rangle| \leq \|\phi\|\,\|\eta\| \leq \|\phi\|\,\|\eta\|_+, \qquad \forall \eta \in \mathcal{H}_b,$$

so that the linear functional $f_\phi : \mathcal{H}_b \to \mathbb{C}$, $f_\phi(\eta) = \langle \phi, \eta\rangle$ is continuous; since $\mathcal{H}_b$ is a Hilbert space, by Riesz's Theorem 1.1.40 there is a unique $\phi_b \in \mathcal{H}_b$ with

$$\langle \phi, \eta\rangle = \langle \phi_b, \eta\rangle_+, \qquad \forall \eta \in \mathcal{H}_b.$$

The last relation will be crucial in what follows.

We then define a linear map $M : \mathcal{H} \to \mathcal{H}_b$, $M\phi := \phi_b$; since dom b is dense in $\mathcal{H}$, note that if $\phi_b = 0$, then $\langle \phi, \eta\rangle = 0, \forall \eta \in \mathcal{H}_b$, and so $\phi = 0$. Hence M is invertible, and for M^{-1} : dom M^{-1} = rng $M \to \mathcal{H}$ write $M^{-1}\phi_b = \phi$, and note that rng $M^{-1} = \mathcal{H}$. Further, since $\|f_\phi\| \leq \|\phi\|$ and, by Riesz $\|f_\phi\| = \|\phi_b\|_+$, it is found that $\|M\phi\|_+ = \|\phi_b\|_+ \leq \|\phi\|$. Thus, M is bounded (with domain $\mathcal{H}$) with norm ≤ 1.

Now it will be shown that rng M is dense in $\mathcal{H}$. Since rng $M \subset$ dom b and $\|\cdot\| \leq \|\cdot\|_1$, it is enough to show that rng $M \sqsubseteq \mathcal{H}_b$. If $\eta \in \mathcal{H}_b$ and $\langle M\xi, \eta\rangle_+ = 0$, $\forall \xi \in \mathcal{H}$, then, by the above crucial relation,

$$0 = \langle M\xi, \eta\rangle_+ = \langle \xi_b, \eta\rangle_+ = \langle \xi, \eta\rangle,$$

and so $\eta = 0$, which proves that density.

The operator M^{-1} is directly related to T_b. Indeed, if $\xi_b \in$ dom M^{-1}, then for all $\eta \in$ dom b,

$$\langle \eta, M^{-1}\xi_b\rangle = \langle \eta, \xi\rangle = \langle \eta, \xi_b\rangle_+ = b(\eta, \xi_b) + (1-\beta)\langle \eta, \xi_b\rangle,$$

or

$$b(\eta, \xi_b) = \langle \eta, M^{-1}\xi_b\rangle - (1-\beta)\langle \eta, \xi_b\rangle = \langle \eta, Q\xi_b\rangle,$$

where $Q := M^{-1} - (1-\beta)\mathbf{1}$, with dom Q = dom M^{-1}. Hence, $\xi_b \in$ dom T_b and $T_b\xi_b = Q\xi_b$; in other words, $Q \subset T_b$. From this relation one infers that T_b is densely defined (because dom Q is dense in $\mathcal{H}$), so hermitian, and the operator Q is also hermitian (because it has a hermitian extension T_b).

Observe that $M^{-1} = Q + (1-\beta)\mathbf{1}$ is also hermitian, and a simple exercise shows that M is also hermitian; since M is bounded ($M \in \mathrm{B}(\mathcal{H})$), it is in fact self-adjoint. By Lemma 2.4.1 one infers that M^{-1} is self-adjoint, so Q is also self-adjoint (very general arguments appear in Theorem 6.1.8 and Exercise 6.1.11). Finally, the relation $Q \subset T_b$ implies $Q = T_b$, since a self-adjoint operator has no proper hermitian extension. The self-adjointness of T_b is hereby verified.

Recall that it was shown above that dom T_b = dom Q = rng M is dense in $\mathcal{H}_b$, that is, dom T_b is a form core of b.

For the uniqueness, suppose that S is self-adjoint with dom $S \subset$ dom b and

$$b(\eta, \xi) = \langle \eta, S\xi\rangle, \qquad \forall \eta \in \text{dom } b,\ \xi \in \text{dom } S.$$

By construction (Definition 4.2.5), $\xi \in \mathrm{dom}\, T_b$ and $T_b\xi = S\xi$; thus $S \subset T_b$. Since S is self-adjoint it has no proper hermitian extension; it then follows that $S = T_b$. □

Exercise 4.2.7. Show that if a linear invertible operator is hermitian, then its inverse is also hermitian.

Exercise 4.2.8. Adapt the statement and proof of Theorem 4.2.6 to the case $b \geq \beta > 0$ and $(\mathrm{dom}\, b, b)$ is complete; in this case write $\mathcal{H}_b$ for $(\mathrm{dom}\, b, b)$ and note that with such approach the inner product $\langle \cdot, \cdot \rangle_+$ does not play any role. Show, in particular, that $\mathrm{dom}\, T_b$ (T_b is the resulting self-adjoint operator, of course) is a form core of b.

Now the hypothesis of $(\mathrm{dom}\, b, b(\cdot, \cdot))$ being closed in Theorem 4.2.6 will be replaced by the assumption that its completion b_+ is compatible with the original Hilbert space $\mathcal{H}$.

Theorem 4.2.9. *Let b be a hermitian sesquilinear form with $b \geq \beta$ for some $\beta \in \mathbb{R}$, its completion $(\mathcal{H}_+, b_+)$ as above and T_{b_+} the self-adjoint operator associated with b_+.*

If b_+ is compatible with $\mathcal{H}$, then there exists a unique self-adjoint operator $\tilde{T}_b : \mathrm{dom}\, \tilde{T}_b \sqsubseteq \mathcal{H}_+ \to \mathcal{H}$, with

$$b(\eta, \xi) = \langle \eta, \tilde{T}_b \xi \rangle, \qquad \forall \eta \in \mathrm{dom}\, b,\ \forall \xi \in \mathrm{dom}\, \tilde{T}_b \cap \mathrm{dom}\, b.$$

Further, $\tilde{T}_b \geq \beta \mathbf{1}$, $\mathrm{dom}\, \tilde{T}_b = \mathrm{dom}\, T_{b_+}$, $\tilde{T}_b = T_{b_+} - (1-\beta)\mathbf{1}$ and $\mathrm{dom}\, \tilde{T}_b$ is a form core of b_+. $\mathcal{H}_+$ is called the form domain of $\tilde{T}_b$.

Proof. Recall that

$$\langle \eta, \xi \rangle_+ = b(\eta, \xi) + (1-\beta)\langle \eta, \xi \rangle, \qquad \forall \eta, \xi \in \mathrm{dom}\, b.$$

So $\langle \eta, \eta \rangle_+ \geq \|\eta\|^2$, $\forall \eta \in \mathrm{dom}\, b$, and since b_+ is compatible with $\mathcal{H}$ it follows that, by Lemma 4.2.2,

$$b_+(\eta, \eta) \geq \|\eta\|^2, \qquad \forall \eta \in \mathrm{dom}\, b_+ = \mathcal{H}_+,$$

that is, $b_+ \geq 1$. Since b_+ is closed, by Theorem 4.2.6, there is a unique self-adjoint operator T_{b_+} with domain dense in $\mathcal{H}_+$ and

$$b_+(\eta, \xi) = \langle \eta, T_{b_+} \xi \rangle, \qquad \forall \eta \in \mathcal{H}_+,\ \xi \in \mathrm{dom}\, T_{b_+}.$$

It also follows that $T_{b_+} \geq \mathbf{1}$.

Now define $\tilde{T}_b := T_{b_+} - (1-\beta)\mathbf{1}$, $\mathrm{dom}\, \tilde{T}_b = \mathrm{dom}\, T_{b_+}$, which is also self-adjoint and $\tilde{T}_b \geq \beta \mathbf{1}$. In case $\eta \in \mathrm{dom}\, b$ and $\xi \in \mathrm{dom}\, b \cap \mathrm{dom}\, T_{b_+}$, one has

$$\langle \eta, T_{b_+} \xi \rangle = b_+(\eta, \xi) = \langle \eta, \xi \rangle_+ = b(\eta, \xi) + (1-\beta)\langle \eta, \xi \rangle,$$

and so

$$b(\eta, \xi) = \langle \eta, (T_{b_+} - (1-\beta)\mathbf{1})\xi \rangle = \langle \eta, \tilde{T}_b \xi \rangle;$$

thus $b(\eta, \xi) = \langle \eta, \tilde{T}_b \xi \rangle$, $\forall \eta \in \mathrm{dom}\, b$, $\forall \xi \in \mathrm{dom}\, \tilde{T}_b \cap \mathrm{dom}\, b$.

Next the uniqueness. Suppose that $\tilde{S} : \text{dom}\, \tilde{S} \sqsubseteq \mathcal{H}_+ \to \mathcal{H}$ is a self-adjoint operator with

$$b(\eta, \xi) = \langle \eta, \tilde{S}\xi \rangle, \qquad \forall \eta \in \text{dom}\, b, \forall \xi \in \text{dom}\, \tilde{S} \cap \text{dom}\, b.$$

Define $S := \tilde{S} + (1 - \beta)\mathbf{1}$; note that $\tilde{S} \neq \tilde{T}_b$ iff $S \neq T_{b_+}$. The above condition on $\tilde{S}$ can be rewritten as

$$b_+(\eta, \xi) = \langle \eta, \tilde{S}\xi \rangle + (1 - \beta)\langle \eta, \xi \rangle = \langle \eta, S\xi \rangle,$$

$\forall \eta \in \text{dom}\, b$, $\forall \xi \in \text{dom}\, S \cap \text{dom}\, b$. Since $(\mathcal{H}_+, b_+)$ is complete and S is closed, together with the continuity of the inner product, one gets

$$b_+(\eta, \xi) = \langle \eta, S\xi \rangle, \qquad \forall \eta \in \mathcal{H}_+, \forall \xi \in \text{dom}\, S;$$

but, by construction, this means that $\xi \in \text{dom}\, T_{b_+}$ and $T_{b_+}\xi = S\xi$, that is, $S \subset T_{b_+}$. Since both are self-adjoint $S = T_{b_+}$, so $\tilde{S} = \tilde{T}_b$ and such an operator is unique. Since $\text{dom}\, \tilde{T}_b = \text{dom}\, T_{b_+}$, Theorem 4.2.6 immediately implies that $\text{dom}\, \tilde{T}_b$ is a form core of b_+. □

Remark 4.2.10. Note that Definition 4.2.5 and the relation

$$b(\eta, \xi) = \langle \eta, \tilde{T}_b\xi \rangle, \qquad \forall \eta \in \text{dom}\, b, \forall \xi \in \text{dom}\, \tilde{T}_b \cap \text{dom}\, b,$$

in the statement of Theorem 4.2.6 imply that $\text{dom}\, \tilde{T}_b$ is given by

$$\{\xi \in \mathcal{H}_+ : \exists \zeta \in \mathcal{H} \text{ with } b_+(\eta, \xi) - (1 - \beta)\xi = \langle \eta, \zeta \rangle,\ \forall \eta \in \text{dom}\, b\},$$

and $\tilde{T}_b\xi = \zeta$.

Recall that the quantum kinetic energy operator in $\mathrm{L}^2(\mathbb{R}^n)$ is the operator $H_0 = -\Delta$ with $\text{dom}\, H_0 = \mathcal{H}^2(\mathbb{R}^n)$ and both $C_0^\infty(\mathbb{R}^n), \mathcal{S}(\mathbb{R}^n)$ are cores of H_0; the laplacian Δ is obtained through distributional derivatives and $\mathcal{H}^2$ is a Sobolev space. Below ∇ indicates the distributional gradient operator.

Example 4.2.11. Let $\text{dom}\, b = \mathcal{H}^1(\mathbb{R}^n) \sqsubseteq \mathrm{L}^2(\mathbb{R}^n)$,

$$b(\phi, \psi) := \langle \nabla\phi, \nabla\psi \rangle, \qquad \phi, \psi \in \text{dom}\, b.$$

Since $b(\phi) = \|\nabla\phi\|^2$, the hermitian sesquilinear form b is positive. Let $(\phi_j) \subset \text{dom}\, b$ be a sequence obeying $b(\phi_j - \phi_k) \to 0$ and $\phi_j \to \phi$ in $\mathrm{L}^2(\mathbb{R}^n)$ as $j, k \to \infty$. Note that this is equivalent to $\phi_j \to \phi$ in $\mathcal{H}^1(\mathbb{R}^n)$, which is a Hilbert space and so $\phi \in \text{dom}\, b$; hence the form b is also closed and $(\text{dom}\, b, \langle\cdot,\cdot\rangle_+)$, with $\langle \phi, \psi \rangle_+ = b(\phi, \psi) + \langle \phi, \psi \rangle$, is a Hilbert space ($\mathcal{H}^1(\mathbb{R}^n)$ in fact!).

It is easily checked that the subsequent self-adjoint operator T_b in Theorem 4.2.6 is H_0; indeed, H_0 is positive and self-adjoint, $\text{dom}\, H_0 = \mathcal{H}^2(\mathbb{R}^n) \sqsubseteq \text{dom}\, b$ and on integrating by parts

$$b(\phi, \psi) = \langle \phi, -\Delta\psi \rangle, \qquad \forall \phi \in \text{dom}\, b, \psi \in \text{dom}\, H_0.$$

Hence, $\mathcal{H}^1(\mathbb{R}^n)$ is the form domain of H_0 and both $C_0^\infty(\mathbb{R}^n), \mathcal{S}(\mathbb{R}^n)$ are form cores of b (since these sets are dense in $\mathcal{H}^1(\mathbb{R}^n)$). In summary, $T_b = H_0$. Usually such form b is denoted by b^{H_0}.

Example 4.2.12. Consider the Hilbert space $\mathcal{H} = \mathrm{L}^2[0,1]$. Let $\alpha = (\alpha_0, \alpha_1)$, $\alpha_0 > 0, \alpha_1 > 0$ (for simplicity), dom $b_\alpha = \mathcal{H}^1[0,1]$ and, for $\phi, \psi \in$ dom b_α,

$$b_\alpha(\phi,\psi) := \langle \phi', \psi' \rangle + \alpha_0\, \overline{\phi(0)}\psi(0) + \alpha_1\, \overline{\phi(1)}\psi(1),$$

which is a densely defined sesquilinear form. For (say!) $a > 1$, integrations by parts show the validity of the integral representations

$$\psi(1) = \int_0^1 t^a \psi'(t)\, dt + \int_0^1 a t^{a-1}\psi(t)\, dt,$$
$$\psi(0) = \int_0^1 -(1-t)^a \psi'(t)\, dt + \int_0^1 a(1-t)^{a-1}\psi(t)\, dt,$$

and by Cauchy-Schwarz,

$$\begin{aligned} b_\alpha(\psi) &\geq \|\psi'\|^2 - \alpha_0\, |\psi(0)|^2 - \alpha_1\, |\psi(1)|^2 \\ &\geq \left(1 - \frac{\alpha_0 + \alpha_1}{2a+1}\right) \|\psi'\|^2 - (\alpha_0 + \alpha_1)\frac{a^2}{2a-1}\|\psi\|^2, \end{aligned}$$

and for a large enough the coefficient of $\|\psi'\|^2$ becomes positive so that $b_\alpha(\psi) \geq \beta\|\psi\|^2$, with $\beta = -(\alpha_0 + \alpha_1)a^2/(2a-1)$. In other words, b_α is lower bounded.

Now it will be argued that b_α is closed, so that it defines a self-adjoint operator T_{b_α} as in Theorem 4.2.6. Let (ψ_n) be a sequence in dom b_α with $b_\alpha(\psi_n - \psi_m) \to 0$ and $\psi_n \to \psi$ in $\mathcal{H}$ as $n, m \to \infty$. Write out such conditions to get that (ψ_n') is also a Cauchy sequence in $\mathcal{H}$ and so $\psi_n' \to \phi \in \mathcal{H}$ (note that $(\psi_n(0))$ and $(\psi_n(1))$ are Cauchy in $\mathbb{C}$). The relation (recall that on bounded intervals convergence in L^2 implies convergence in L^1)

$$\int_0^t \phi(s)\, ds = \lim_{n\to\infty} \int_0^t \psi_n'(s)\, ds = \psi(t) - \psi(0)$$

implies that $\psi \in$ dom b_α and $\psi' = \phi$. By continuity of the elements of $\mathcal{H}^1[0,1]$ and the above integral representations for $\psi_n(0), \psi_n(1)$, one has $\psi_n(0) \to \psi(0)$ and $\psi_n(1) \to \psi(1)$. A direct verification that $b_\alpha(\psi_n - \psi) \to 0$ concludes that b_α is closed.

The next step is to find T_{b_α} via $b_\alpha(\phi,\psi) = \langle \phi, T_{b_\alpha}\psi \rangle$. After a formal integration by parts in the expression of $b_\alpha(\phi,\psi)$ one gets

$$\begin{aligned} \langle \phi, T_{b_\alpha}\psi \rangle &= b_\alpha(\phi,\psi) \\ &= \langle \phi, -\psi'' \rangle + \overline{\phi(0)}\,(\alpha_0\psi(0) + \psi'(0)) - \overline{\phi(1)}(\alpha_1\psi(1) - \psi'(1)), \end{aligned}$$

which suggests to try dom $T_{b_\alpha} = \{\psi \in \mathcal{H}^2[0,1] : \psi'(0) = -\alpha_0\psi(0), \psi'(1) = \alpha_1\psi(1)\}$, $T_{b_\alpha}\psi = -\psi''$. One can check that this operator T_{b_α} is actually self-adjoint; since dom $T_{b_\alpha} \sqsubseteq$ dom b_α and

$$b_\alpha(\phi, \psi) = \langle \phi, T_{b_\alpha}\psi\rangle, \qquad \forall \phi \in \text{dom } b_\alpha, \psi \in \text{dom } T_{b_\alpha},$$

one has that T_α is the operator associated with the form b_α in Theorem 4.2.6, and $\mathcal{H}^1[0,1]$ is the form domain of T_α.

Exercise 4.2.13. Verify that T_{b_α} in Example 4.2.12 is self-adjoint (a possible solution can be obtained from a characterization in Example 7.3.4).

Exercise 4.2.14. Consider the Hilbert space $\mathcal{H} = \mathrm{L}^2[0,1]$, dom $\tilde{b} = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$ and, for $\phi, \psi \in$ dom $\tilde{b}$,

$$\tilde{b}(\phi, \psi) = \langle \phi', \psi'\rangle.$$

Based on Example 4.2.12, show that $\tilde{b}$ is a positive closed form whose corresponding associated operator is dom $T_{\tilde{b}} = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}$, $T_{\tilde{b}}\psi = -\psi''$, $\psi \in$ dom $T_{\tilde{b}}$.

Let b_1, b_2 be two closed and lower bounded forms and T_{b_1}, T_{b_2} the subsequent self-adjoint operators associated with b_1 and b_2, respectively. It can happen that the sesquilinear form sum $b = b_1 + b_2$, with dom $(b_1 + b_2) =$ dom $b_1 \cap$ dom b_2, is either closed and lower bounded or its completion b_+ is compatible with the original Hilbert space; in either way the operator T_b associated with b is self-adjoint and called the *form sum* of T_{b_1} and T_{b_2}, and denoted by

$$T_b = T_{b_1} \dot{+} T_{b_2}.$$

This concept is illustrated in the following example; see also Subsection 6.1.1 and Remark 9.3.13.

Example 4.2.15. Let T_α, $\alpha = (\alpha_0, \alpha_1)$, be the operator obtained in Example 4.2.12, and consider also T_τ, $\tau = (\tau_0, \tau_1)$, obtained in the same way. The aim here is to describe the operator $T_\alpha/2 \dot{+} T_\tau/2$. First note that $T_\alpha/2$ is the operator associated with the form $b_\alpha/2$.

Let $b = b_\alpha/2 + b_\tau/2$, i.e., dom $b = \mathcal{H}^1[0,1]$,

$$b(\phi, \psi) = \langle \phi', \psi'\rangle + \frac{\alpha_0 + \tau_0}{2}\overline{\phi(0)}\,\psi(0) + \frac{\alpha_1 + \tau_1}{2}\,\overline{\phi(1)}\psi(1),$$

consequently

$$\frac{T_\alpha}{2} \dot{+} \frac{T_\tau}{2} = T_\omega, \qquad \omega = \left(\frac{\alpha_0 + \tau_0}{2}, \frac{\alpha_1 + \tau_1}{2}\right).$$

See also Example 4.4.8.

4.3 Friedrichs Extension

Given T hermitian, consider the form generated by T, that is, $b^T(\xi,\eta) = \langle \xi, T\eta\rangle$, $\xi,\eta \in \text{dom } T$; if $T \geq \beta\mathbf{1}$, one has $b^T(\xi,\xi) \geq \beta\|\xi\|^2$, and it is possible to apply Theorem 4.2.9 in order to get the so-called Friedrichs extension of T (a fundamental result by Friedrichs of 1934).

Theorem 4.3.1 (Friedrichs Extension). *Let T be a lower bounded hermitian operator with $T \geq \beta\mathbf{1}$, $\beta \in \mathbb{R}$, b^T the form generated by T, i.e.,*

$$b^T(\xi,\eta) = \langle \xi, T\eta\rangle, \qquad \xi,\eta \in \text{dom } b^T = \text{dom } T,$$

and $(\mathcal{H}_+^T, b_+^T)$ as in Example 4.2.4. Then the operator T has a unique self-adjoint extension $T_F : \text{dom } T_F \to \mathcal{H}$ with $\text{dom } T_F \sqsubseteq \mathcal{H}_+^T$. Further, $T_F \geq \beta\mathbf{1}$ and $\text{dom } T_F$ is a form core of b_+^T. $\mathcal{H}_+^T$ is the form domain of T_F.

Proof. Recall that $\langle \xi,\eta\rangle_+ = b^T(\xi,\eta) + (1-\beta)\langle \xi,\eta\rangle$, $\xi,\eta \in \text{dom } T$, and its completion is $(\mathcal{H}_+^T, b_+^T)$. On account of Example 4.2.4, b_+^T is compatible with $\mathcal{H}$ and $b_+^T(\xi,\xi) \geq \|\xi\|^2$, $\forall \xi \in \mathcal{H}_+^T$. By Theorem 4.2.9 there is a unique self-adjoint operator

$$T_F = \tilde{T}_{b^T} := T_{b_+^T} - (1-\beta)\mathbf{1}, \qquad \text{dom } T_F = \text{dom } T_{b_+^T} \sqsubseteq \mathcal{H}_+^T,$$

so that

$$b^T(\eta,\xi) = \langle \eta, T_F\xi\rangle, \qquad \forall \eta \in \text{dom } T,\ \xi \in \text{ dom } T \cap \text{dom } T_F.$$

Since $T_{b_+^T} \geq \mathbf{1}$ one finds that $T_F \geq \beta\mathbf{1}$. In order to show that $T \subset T_F$, take note initially that for $\xi,\eta \in \text{dom } T$,

$$b_+^T(\eta,\xi) = \langle \eta,\xi\rangle_+ = \langle \eta, [T + (1-\beta)\mathbf{1}]\xi\rangle\,.$$

By continuity of the inner product, density of $\text{dom } T$ in $\mathcal{H}_+^T$ and the continuity of the inclusion $j : \mathcal{H}_+^T \to \mathcal{H}$, it follows that, for each $\xi \in \text{dom } T$,

$$b_+^T(\eta,\xi) = \langle \eta, [T + (1-\beta)\mathbf{1}]\xi\rangle$$

holds true for any $\eta \in \mathcal{H}_+^T$. Hence, by the construction in Definition 4.2.5, $\xi \in \text{dom } T_{b_+^T}$ and $T_{b_+^T}\xi = T\xi + (1-\beta)\xi$, showing that

$$T\xi = T_{b_+^T}\xi - (1-\beta)\xi = T_F\xi, \qquad \forall \xi \in \text{dom } T.$$

Hence $T \subset T_F$.

Now the uniqueness of T_F. If S is a self-adjoint operator so that $T \subset S$ and $\text{dom } S \subset \mathcal{H}_+^T$, the above proof that $T \subset T_F$ applies, and so one concludes that $S \subset T_F$; since both operators are self-adjoint, $S = T_F$. As in Theorem 4.2.6, one concludes that $\text{dom } T_F$ is a form core of b_+^T. □

Exercise 4.3.2. Conclude that (see Remark 4.2.10) dom T_F is given by

$$\left\{\xi \in \mathcal{H}_+^T : \exists \zeta \in \mathcal{H} \text{ with } b_+^T(\xi,\eta) - (1-\beta)\langle \xi,\eta\rangle = \langle \zeta,\eta\rangle,\ \forall \eta \in \text{dom } T\right\},$$

and $T_F\xi = \zeta$. Given $\xi \in \text{dom } T_F$, by taking $(\xi_n) \subset \text{dom } T$ with $\xi_n \to \xi$ in $\mathcal{H}_+^T$, show that

$$\begin{aligned} b_+^T(\xi,\eta) - (1-\beta)\langle \xi,\eta\rangle &= \lim_{n\to\infty} [b_+^T(\xi_n,\eta) - (1-\beta)\langle \xi_n,\eta\rangle] \\ &= \langle \xi, T\eta\rangle, \qquad \forall \eta \in \text{dom } T, \end{aligned}$$

and conclude that dom T_F = dom $T^* \cap \mathcal{H}_+^T$.

Definition 4.3.3. The self-adjoint operator T_F introduced in Theorem 4.3.1 is called the Friedrichs extension of the hermitian and lower bounded T.

Proposition 4.3.4. *Let $T \geq \beta\mathbf{1}$ and T_0 a lower bounded self-adjoint extension of T. Then $\mathcal{H}_+^{T_F} \subset \mathcal{H}_+^{T_0}$, that is, the Friedrichs extension has the smallest form domain among the form domains of lower bounded self-adjoint extensions of T.*

Proof. Assume that β is the largest lower bound of T and let $\alpha \in \mathbb{R}$ be strictly less than a lower bound of T_0; so $\alpha < \beta$.

It is known that the form domain $\mathcal{H}_+^{T_F}$ of T_F is the completion of dom T in the norm $\langle \xi,\xi\rangle_+ = \langle \xi, [T + (1-\beta)\mathbf{1}]\xi\rangle$, which is the same space obtained after completion of dom T in the norm

$$\langle \xi, [T + (1-\alpha)\mathbf{1}]\xi\rangle = \langle \xi, [T_0 + (1-\alpha)\mathbf{1}]\xi\rangle.$$

Since dom $T \subset$ dom T_0 and the form domain $\mathcal{H}_+^{T_0}$ of T_0 is the completion of dom T_0 in the above norm $\langle \xi, [T_0 + (1-\alpha)\mathbf{1}]\xi\rangle$, it follows that $\mathcal{H}_+^{T_F} \subset \mathcal{H}_+^{T_0}$. □

It is interesting to point out that T_F is the only self-adjoint extension of T whose domain is dense in $\mathcal{H}_+^T$; particularly, the only self-adjoint extension whose form domain is $\mathcal{H}_+^T$. Thus, in this sense and in view of Proposition 4.3.4, T_F is canonically constructed.

Corollary 4.3.5. *If T is hermitian and lower bounded, then its deficiency indices are equal.*

Proof. T_F is a self-adjoint extension of the operator T. Now apply Theorem 2.2.11. □

Exercise 2.4.17 implies an important lower bound of the spectrum of the Friedrichs extension:

Corollary 4.3.6. *Let $T \geq \beta$ be as in Theorem* 4.3.1 *and T_F the consequent Friedrichs extension. Then $\sigma(T_F) \subset [\beta,\infty)$.*

However, Example 4.4.13 presents another self-adjoint extension of a lower bounded hermitian operator T with the same spectrum of T_F.

In case the Hilbert space is $\mathrm{L}^2(\mathbb{R}^n)$, one can anticipate an important result if Corollary 6.3.5 is invoked:

Corollary 4.3.7. *If there is $\beta \in \mathbb{R}$ so that $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$ satisfies $V(x) \geq \beta$, $\forall x \in \mathbb{R}^n$, then the Friedrichs extension of the standard Schrödinger operator*

$$\mathrm{dom}\ H = C_0^\infty(\mathbb{R}^n), \qquad H\psi = -\Delta\psi + V\psi, \quad \psi \in \mathrm{dom}\ H,$$

is the unique self-adjoint extension of H.

If $T \in \mathrm{B}(\mathcal{H})$, then T^*T is self-adjoint and positive. Form extensions will be used to adapt this result to a more general case. Recall that $\mathrm{dom}\ (T^*T) := \{\xi \in \mathrm{dom}\ T : (T\xi) \in \mathrm{dom}\ T^*\}$ and $(T^*T)\xi = T^*(T\xi)$. However, it can happen that $\mathrm{dom}\ (T^*T)$ is not dense in $\mathcal{H}$. See Example 2.1.5; another classical example is the following.

Example 4.3.8 (dom T^* is not dense in $\mathcal{H}$)*.* Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R})$, $0 \neq \psi_0 \in \mathcal{H}$, $\phi(x) = 1, \forall x \in \mathbb{R}$ and $\mathrm{dom}\ T := \{\psi \in \mathcal{H} : \int_{\mathbb{R}} |\psi| dx < \infty\}$. Write $\langle \phi, \psi \rangle = \int_{\mathbb{R}} \psi dx$, and define

$$(T\psi)(x) := \langle \phi, \psi \rangle \psi_0(x), \qquad \psi \in \mathrm{dom}\ T.$$

Thus, if $u \in \mathrm{dom}\ T^*$, then for every $\psi \in \mathrm{dom}\ T$ one has

$$\begin{aligned} \langle T^*u, \psi \rangle &= \langle u, T\psi \rangle = \langle u, \langle \phi, \psi \rangle \psi_0 \rangle \\ &= \langle \phi, \psi \rangle \langle u, \psi_0 \rangle = \langle \langle \psi_0, u \rangle \phi, \psi \rangle . \end{aligned}$$

Hence, $(T^*u)(x) = \langle \psi_0, u \rangle \phi(x)$, and it belongs to $\mathcal{H}$ iff $\langle \psi_0, u \rangle = 0$. Thus, $\mathrm{dom}\ T^* \subset \{\psi_0\}^\perp$ and it is not dense in $\mathcal{H}$. Furthermore, for $u \in \mathrm{dom}\ T^*$ one has $T^*u = 0$.

However, if T is closed a remarkable result of von Neumann is found.

Proposition 4.3.9. *Let T be a closed operator with* dom $T \sqsubseteq \mathcal{H}$*. Then* dom $(T^*T) \sqsubseteq \mathcal{H}$*, T^*T is a positive self-adjoint operator and* dom T *is the form domain of T^*T.*

Proof. Since T is closed, by taking the form

$$b(\xi, \eta) := \langle \xi, \eta \rangle_T = \langle T\xi, T\eta \rangle + \langle \xi, \eta \rangle$$

as the inner graph product, it follows that $(\mathcal{H}_+, b_+) = (\mathrm{dom}\ T, b)$ is a Hilbert space and $b(\xi) = \|\xi\|_T \geq \|\xi\|$, $\forall \xi \in \mathrm{dom}\ T$. Thus, by Theorem 4.2.6 the operator T_b associated with b is self-adjoint, $T_b \geq \mathbf{1}$,

$$\mathrm{dom}\ T_b = \{\xi \in \mathrm{dom}\ T : \exists \phi \in \mathcal{H} \text{ with } b(\eta, \xi) = \langle \eta, \phi \rangle, \forall \eta \in \mathrm{dom}\ T\}$$

and $T_b\xi = \phi$. Explicitly, $\xi \in \mathrm{dom}\ T_b$ iff for all $\eta \in \mathrm{dom}\ T$,

$$\langle T\eta, T\xi \rangle + \langle \eta, \xi \rangle = b(\eta, \xi) = \langle \eta, T_b\xi \rangle,$$

so that

$$\langle T\eta, T\xi \rangle = \langle \eta, (T_b - \mathbf{1})\xi \rangle, \qquad \forall \eta \in \mathrm{dom}\ T.$$

Therefore, $\xi \in \mathrm{dom}\ T_b$ iff $T\xi \in \mathrm{dom}\ T^*$ and $T^*(T\xi) = (T_b - \mathbf{1})\xi$, that is, $T^*T = T_b - \mathbf{1}$ is self-adjoint and positive. By Theorem 4.2.6, $\mathrm{dom}\ T_b$ is dense in $(\mathrm{dom}\ T, b)$, and it follows that $\mathrm{dom}\ (T^*T)$ is dense in $(\mathrm{dom}\ T, b)$. By construction, the form domain of T^*T is $\mathrm{dom}\ T$. □

Although the next result could be obtained directly from general theorems, it is worth presenting a specific short proof.

Corollary 4.3.10. *If T is self-adjoint, then for all $n \in \mathbb{N}$ the operator T^{2^n} is positive and self-adjoint. In particular T^2 is self-adjoint.*

Proof. If T^j is self-adjoint, Proposition 4.3.9 implies that T^{2j} is self-adjoint; use recursion in j starting from $j = 1$. □

Proposition 4.3.11. *Let T be closed and densely defined.*

i) *Then* dom (T^*T) *is a core of T.*
ii) *If T is self-adjoint, then T^2 is self-adjoint and* dom T^2 *is a core of T.*

Proof. i) In the graph inner product of T, let

$$(\eta, T\eta) \in \{(\xi, T\xi) : \xi \in \mathrm{dom}\ (T^*T)\}^{\perp}.$$

Thus $0 = \langle \xi, \eta \rangle + \langle T\xi, T\eta \rangle = \langle (\mathbf{1} + T^*T)\xi, \eta \rangle$. Since T^*T is a positive self-adjoint operator, $-1 \in \rho(T^*T)$ and so rng $(T^*T + \mathbf{1}) = \mathcal{H}$. Hence $\eta = 0$ and, by Exercise 1.2.26 (or Exercise 2.5.10), dom (T^*T) is a core of T.

ii) Combine Corollary 4.3.10 with i). □

Remark 4.3.12. The following property is attractive. If T is self-adjoint and dom $T^2 =$ dom T, then T is bounded.

Proof. Clearly dom $T^2 \subset$ dom T and we introduce the notation $\mathbf{h} = (\mathrm{dom}\ T, \|\cdot\|_T)$, which is a Hilbert space since T is closed. Pay attention to the following facts:

1. $T - i\mathbf{1} : \mathbf{h} \to (\mathcal{H}, \|\cdot\|)$ is bounded. Indeed, for $\xi \in$ dom T, $\|(T - i\mathbf{1})\xi\|^2 = \|\xi\|^2 + \|T\xi\|^2 = \|\xi\|_T^2$.
2. Since dom $T^2 =$ dom T one has Tdom $T \subset$ dom T and so the linear mapping

$$R_i(T) : (\mathrm{dom}\ T, \|\cdot\|) \to \mathbf{h}$$

is bounded. Indeed, for $\xi \in$ dom T use triangular inequality to get

$$\begin{aligned}\|R_i(T)\xi\|_T^2 &= \|R_i(T)\xi\|^2 + \|TR_i(T)\xi\|^2 \\ &\le \|\xi\|^2 + \|(T - i\mathbf{1})R_i(T)\xi + iR_i(T)\xi\|^2 \le 5\|\xi\|^2.\end{aligned}$$

3. Since dom $T^2 =$ dom T, define

$$\tilde{T} : \mathbf{h} \to \mathbf{h}, \qquad \tilde{T}\xi := T\xi,$$

which is a closed operator; indeed, if $\xi_n \xrightarrow{\mathbf{h}} \xi$ and $T\xi_n \xrightarrow{\mathbf{h}} \eta$, then $\xi \in$ dom T, $T\xi_n \xrightarrow{\mathcal{H}} T\xi$, $T\xi_n \xrightarrow{\mathcal{H}} \eta$, so that $\eta = T\xi$. Hence, $\tilde{T}$ is bounded by the closed graph theorem.

Now observe that $T : (\text{dom } T, \|\cdot\|) \to (\mathcal{H}, \|\cdot\|)$ can be written in the form

$$T = (T - i\mathbf{1})\,\tilde{T}\,R_i(T),$$

which shows that T is bounded. □

Exercise 4.3.13. Let T be a closed hermitian operator with dom T^2 dense in $\mathcal{H}$. Show that T^*T is the Friedrichs extension of T^2.

Exercise 4.3.14. Let dom $a = \{\psi \in \mathrm{L}^2(\mathbb{R}) : \psi \in \mathrm{AC}(\mathbb{R}), \psi' + x\psi \in \mathrm{L}^2(\mathbb{R})\}$, $a\psi = \psi' + x\psi$, $\psi \in$ dom a. Show that a is a closed operator and that its adjoint is dom $a^* = \{\psi \in \mathrm{L}^2(\mathbb{R}) : \psi \in \mathrm{AC}(\mathbb{R}), -\psi' + x\psi \in \mathrm{L}^2(\mathbb{R})\}$, $a^*\psi = -\psi' + x\psi$, $\psi \in$ dom a^*. Find the operator a^*a and relate it to the harmonic oscillator. a^*, a are called *creation* and *annihilation* operators, respectively.

Exercise 4.3.15. If T is self-adjoint and E is a dense subspace of $\mathcal{H}$, show that $R_i(T)E$ is also dense in $\mathcal{H}$. Observe that dom $T^{n+1} = R_i(T)$dom T^n for all $n \in \mathbb{N}$, and conclude that dom T^n is dense in $\mathcal{H}$.

Exercise 4.3.16. Let T be a closed operator with dom $T \sqsubseteq \mathcal{H}$. Choose $\xi' = 0$ in Exercise 2.1.21 and work to show that $(\mathbf{1} + T^*T)^{-1}$ is a bounded self-adjoint operator. Conclude that T^*T is self-adjoint. This is a sketch of a proof of the first part of Proposition 4.3.9 without using forms.

4.4 Examples

Example 4.4.1. Let $\varphi : \mathbb{R} \to [0, \infty)$ be a Borel function and $T = \mathcal{M}_\varphi \geq 0$ the subsequent self-adjoint multiplication operator in $\mathrm{L}^2(\mathbb{R})$, as in Subsection 2.3.2. The sesquilinear form generated by T is dom $b^T =$ dom $\mathcal{M}_\varphi$,

$$b^T(\psi, \phi) = \langle \psi, \mathcal{M}_\varphi \phi \rangle = \int_{\mathbb{R}} \overline{\psi(x)}\,\varphi(x)\phi(x)\,dx.$$

By writing

$$b^T(\psi, \phi) = \int_{\mathbb{R}} \overline{\varphi(x)^{\frac{1}{2}}\psi(x)}\;\varphi(x)^{\frac{1}{2}}\phi(x)\,dx$$

one has

$$\langle \psi, \phi \rangle_+ = \langle \mathcal{M}_{\sqrt{\varphi}}\psi, \mathcal{M}_{\sqrt{\varphi}}\phi \rangle + \langle \psi, \phi \rangle, \qquad \psi, \phi \in \text{dom } T,$$

which is the graph inner product of $\mathcal{M}_{\sqrt{\varphi}}$ restricted to dom T. Now, it is possible to show (Lemma 4.4.2) that dom $\mathcal{M}_\varphi$ is dense in dom $\mathcal{M}_{\sqrt{\varphi}}$ and since the operator $\mathcal{M}_{\sqrt{\varphi}}$ is closed, it follows that $b^T_+ = \langle \cdot, \cdot \rangle_+$ and $\mathcal{H}^T_+$ is the domain of $\mathcal{M}_{\sqrt{\varphi}}$. In summary, the form domain of the positive self-adjoint operator $\mathcal{M}_\varphi$ (so equal to its Friedrichs extension) is dom $\mathcal{M}_{\sqrt{\varphi}}$. Note that, for general function φ, dom $T =$ dom $\mathcal{M}_\varphi$ is a proper subset of $\mathcal{H}^T_+ =$ dom $\mathcal{M}_{\sqrt{\varphi}}$. Later on this will be generalized (see Section 9.3).

Lemma 4.4.2. *Consider all symbols as in Example* 4.4.1. *In both spaces,* $\mathcal{H}$ *and* $\mathcal{H}_+ = (\mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}, \langle\cdot,\cdot\rangle_{\mathcal{M}_{\sqrt{\varphi}}})$*, one has* $\mathrm{dom}\ \mathcal{M}_\varphi \sqsubseteq \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$ *(see also general arguments in Proposition* 4.3.11*).*

Proof. If $\psi \in \mathrm{dom}\ \mathcal{M}_\varphi$ then, by Cauchy-Schwarz,

$$\|\sqrt{\varphi}\psi\|^2 = \int_E \overline{\psi(x)}\,\varphi(x)\,\psi(x)\,d\mu(x) \le \|\psi\|\|\varphi\psi\| < \infty,$$

and $\mathrm{dom}\ \mathcal{M}_\varphi \subset \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$.

Given $\psi \in \mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$, for each positive integer n set $E_n = \{x \in E : 0 \le \varphi(x) \le n\}$ and $\psi_n(x) = \chi_{E_n}(x)\psi(x)$. Then $\psi_n \in \mathrm{dom}\ \mathcal{M}_\varphi$ and

$$\|\sqrt{\varphi}\,(\psi_n - \psi)\|^2 = \int_E \varphi(x)\,|1 - \chi_{E_n}(x)|^2\ |\psi(x)|^2\,d\mu(x)$$

which vanishes as $n \to \infty$, by the dominated convergence theorem. In a similar way one checks that $\psi_n \to \psi$ in $\mathcal{H}$, that is, in this space $\mathrm{dom}\ \mathcal{M}_\varphi$ is dense in $\mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$.

Taking these two convergences together, it follows that

$$\|\psi_n - \psi\|_+^2 = \|\sqrt{\varphi}\,(\psi_n - \psi)\|^2 + \|\psi_n - \psi\|^2 \overset{n\to\infty}{\longrightarrow} 0,$$

which shows that $\mathrm{dom}\ \mathcal{M}_\varphi$ is dense in $\mathrm{dom}\ \mathcal{M}_{\sqrt{\varphi}}$ in $\mathcal{H}_+$. □

The next examples indicate that occasionally the Friedrichs extension naturally allocates boundary conditions.

Example 4.4.3. Let $\mathrm{dom}\ P = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$, $P\psi = -i\psi'$, and $H = P^2$, with

$$\begin{aligned}\mathrm{dom}\ H &= \{\psi \in \mathrm{dom}\ P : P\psi \in \mathrm{dom}\ P\}\\ &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi(1) = 0 = \psi'(0) = \psi'(1)\},\end{aligned}$$

and $H\psi = -\psi''$. P is a closed hermitian operator and its adjoint has the same action but with domain $\mathrm{dom}\ P^* = \mathcal{H}^1[0,1]$. Therefore, by Proposition 4.3.9, P^*P is self-adjoint,

$$\begin{aligned}\mathrm{dom}\ P^*P &= \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1),\ \psi' \in \mathcal{H}^1[0,1]\}\\ &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}.\end{aligned}$$

By results of Section 4.3, P^*P is the Friedrichs extension of H, i.e., $P^*P = H_F$. This is the unique self-adjoint extension of the free particle energy operator T_D in $[0,1]$, Example 2.3.5, with Dirichlet boundary conditions. This is a general feature of the Friedrichs extension of differential operators, that is, it corresponds to the Dirichlet boundary conditions; see other examples below.

Exercise 4.4.4. Show that the unique self-adjoint extension of the free particle energy operator T_P in $[0,1]$, with periodic boundary conditions of Example 2.3.7, is the Friedrichs extension of P^2, where dom $P = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = \psi(1)\}$, $P\psi = -i\psi'$. Find the domain of this extension.

Example 4.4.5. [Energy operator on $[0,1]$] Set $\mathcal{H} = \mathrm{L}^2[0,1]$, dom $H = C_0^\infty(0,1)$,

$$(H\psi)(x) := -\psi''(x) + V(x)\psi(x),$$

with $V : [0,1] \to [0,\infty)$ continuous. Consider the form generated by this operator, that is, $b^H : \text{dom } H \times \text{dom } H \to \mathbb{C}$, $b^H(\psi,\phi) := \langle \psi, H\phi \rangle$. Thus

$$\begin{aligned} b^H(\psi,\psi) &= \int_0^1 \overline{\psi(x)} \left(-\psi''(x) + V(x)\psi(x)\right) \, dx \\ &= \int_0^1 \left(|\psi'(x)|^2 + V(x)|\psi(x)|^2\right) \, dx \geq \beta \|\psi\|^2, \end{aligned}$$

with $0 \leq \beta = \min_{x\in[0,1]} V(x)$. Thus $H \geq \beta\mathbf{1}$.

Let H_F be the Friedrichs extension of H; so dom $H_F \subset \mathcal{H}_+^H$. For $\psi \in$ dom H, by Cauchy-Schwarz one has

$$\begin{aligned} |\psi(x) - \psi(0)| &= \left| \int_0^x \psi'(t) dt \right| \leq |x|^{\frac{1}{2}} \left(\int_0^x |\psi'(t)|^2 \, dt \right)^{\frac{1}{2}} \\ &\leq |x|^{\frac{1}{2}} \, b^H(\psi,\psi)^{\frac{1}{2}}. \end{aligned}$$

Since $\psi(0) = 0$ one has

$$\|\psi\|_\infty = \sup_{x\in[0,1]} |\psi(x)| \leq b^H(\psi,\psi)^{\frac{1}{2}} \leq \langle \psi, \psi \rangle_+^{\frac{1}{2}};$$

thus each Cauchy sequence according to either $b^H(\cdot,\cdot)$ or $\langle \cdot, \cdot \rangle_+$ norm converges uniformly, and so its limit is also continuous and vanishing at the boundary. Then this holds for every element of the complete space $\mathcal{H}_+^H$, in particular for the elements of dom H_F. Therefore, null Dirichlet boundary conditions $\psi(0) = 0 = \psi(1)$ hold in dom H_F. Note that the result is in fact valid for more general positive potentials $V(x)$.

Exercise 4.4.6. Let $\mathcal{H} = \mathrm{L}^2[0,1]$, $V : [0,1] \to [0,\infty)$ continuous, dom $\underline{b} = \{\psi \in \mathcal{H}^1[0,1] : \psi(0) = 0 = \psi(1)\}$ and, for $\phi, \psi \in$ dom $\underline{b}$,

$$\underline{b}(\phi,\psi) = \langle \phi', \psi' \rangle + \langle \phi, V\psi \rangle$$

Based on Example 4.2.12, show that $\underline{b}$ is a positive closed form whose respective associated operator is dom $T_{\underline{b}} = \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\}$, $T_{\underline{b}}\psi = -\psi'' + V\psi$, $\psi \in$ dom $T_{\underline{b}}$. Show that $\underline{b}$ here is the closure of the form b in Example 4.4.5, and conclude that $T_{\underline{b}}$ is the Friedrichs extension H_F of the operator H in that example.

Example 4.4.7. Let $\mathcal{H} = \mathrm{L}^2[0,1]$, $p, V : [0,1] \to \mathbb{R}$ continuous functions, with $p(x) \geq 0$, $\forall x \in [0,1]$, and continuous derivative p'. Given $a \geq 0$, consider the operator

$$\begin{aligned} \mathrm{dom}\, T &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0,\ \psi'(1) = -a\psi(1)\}, \\ (T\psi)(x) &= -[p\psi']'(x) + V(x)\psi(x), \qquad \psi \in \mathrm{dom}\, T. \end{aligned}$$

Integrations by parts show that T is hermitian, and since

$$\begin{aligned} \langle \psi, T\psi \rangle &= a\, p(1)|\psi(1)|^2 + \int_0^1 p(x)|\psi'(x)|^2\, dx + \int_0^1 V(x)|\psi(x)|^2\, dx \\ &\geq \int_0^1 V(x)|\psi(x)|^2\, dx \geq \beta\|\psi\|^2, \qquad \beta = \inf\{V(x) : x \in [0,1]\}, \end{aligned}$$

it follows that $T \geq \beta\mathbf{1}$. Therefore, this operator has a self-adjoint extension T_F, its Friedrichs extension, and $T_F \geq \beta\mathbf{1}$. In particular $\sigma(T_F) \subset [\beta, \infty)$.

Example 4.4.8. Let T_α, T_τ be operators as introduced in Example 4.2.15 and assume that $\alpha_0 \neq \tau_0$, $\alpha_1 \neq \tau_1$ (recall that they are not zero). Consider the operator sum $(T_\alpha + T_\tau)/2$, whose domain is

$$\begin{aligned} \mathrm{dom}\,(T_\alpha/2) \cap \mathrm{dom}\,(T_\tau/2) = \Big\{ &\psi \in \mathcal{H}^2[0,1] : \\ &\psi'(0) = \frac{\alpha_0}{2}\psi(0) = \frac{\tau_0}{2}\psi(0), \psi'(1) = -\frac{\alpha_1}{2}\psi(1) = -\frac{\tau_1}{2}\psi(1) \Big\} \\ = \{&\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1), \psi'(0) = 0 = \psi'(1)\}. \end{aligned}$$

Since the situation is very similar to Exercise 4.2.14 and Example 4.4.3, one concludes that $(T_\alpha + T_\tau)/2 \geq 0$ and the domain of its Friedrichs extension $((T_\alpha + T_\tau)/2)_F$ carries Dirichlet boundary conditions, i.e., $\psi(0) = 0 = \psi(1)$. Therefore

$$\frac{T_\alpha}{2} \dot{+} \frac{T_\tau}{2} \neq \left(\frac{T_\alpha}{2} + \frac{T_\tau}{2} \right)_F ;$$

see Example 4.2.15.

Example 4.4.9. [Schrödinger operator with delta-function potential] Let $c > 0$ and $\delta(x)$ be the Dirac delta at the origin (see also Example 6.2.16 and Subsection 7.4.2). A way to interpret the formal energy operator (in $\mathrm{L}^2(\mathbb{R})$)

$$T^c = -\frac{d^2}{dx^2} + c\,\delta(x),$$

under this δ potential with positive intensity c, is to consider a suitable domain for T^c, which contains all information on $\delta(x)$, and then construct a self-adjoint extension via sesquilinear forms (see Example 4.1.15). Physically, $\delta(x)$ models a very strong (positive) interaction concentrated at the origin.

As a guide for defining such domain, for $\varepsilon > 0$ integrate $T^c\psi$ formally

$$\int_{-\varepsilon}^{\varepsilon} (T^c\psi)(x)\,dx = \int_{-\varepsilon}^{\varepsilon} -\psi''(x)\,dx + \int_{-\varepsilon}^{\varepsilon} c\,\delta(x)\psi(x)\,dx$$
$$= \psi'(-\varepsilon) - \psi'(\varepsilon) + c\,\psi(0).$$

The term $c\psi(0)$ induces 1. below. If the function $(T^c\psi)$ is bounded (so 3. below), then as $\varepsilon \to 0^+$ one gets

$$0 = \psi'(0^-) - \psi'(0^+) + c\,\psi(0),$$

and so 2. below. Based on this motivating digression, define dom T^c as the set of $\psi \in \mathcal{H}^2(\mathbb{R} \setminus \{0\})$ obeying

1. ψ is continuously extended at zero, that is, $\psi(0^+) = \psi(0^-) := \psi(0)$;
2. $\psi'(0^+) - \psi'(0^-) = c\psi(0)$;
3. $\psi''(0^+) - \psi''(0^-)$ is finite.

This set dom T^c contains $C_0^\infty(\mathbb{R} \setminus \{0\})$ and so is dense in $\mathrm{L}^2(\mathbb{R})$. Finally define

$$T^c\psi := -\psi'', \qquad \psi \in \operatorname{dom} T^c.$$

For $\psi, \phi \in \operatorname{dom} T^c$ one has, after integration by parts,

$$b^{T^c}(\psi,\phi) = \langle \psi, T^c\phi\rangle = -\int_{-\infty}^{0^-} \overline{\psi(x)}\,\phi''(x)\,dx - \int_{0^+}^{\infty} \overline{\psi(x)}\,\phi''(x)\,dx$$
$$= \overline{\psi(0^+)}\,\phi'(0^+) - \overline{\psi(0^-)}\,\phi'(0^-) + \int_{\mathbb{R}} \overline{\psi'(x)}\,\phi'(x)\,dx$$
$$= c\,\overline{\psi(0)}\,\phi(0) + \langle \psi', \phi'\rangle = \langle \psi', \phi'\rangle + c\,b_\delta(\psi,\phi),$$

where b_δ is the form in Example 4.1.15. Two important conclusions follow. First, the form $b^{T^c}(\psi,\phi)$ is the sum

$$b^{T^c}(\psi,\phi) = \langle \psi', \phi'\rangle + c\,b_\delta(\psi,\phi),$$

supporting the interpretation of the presence of a δ potential with intensity $c > 0$. Second, another integration by parts shows that T^c is hermitian, and for $\psi = \phi$ one has

$$\langle \psi, T^c\psi\rangle = c\,|\psi(0)|^2 + \|\psi'\|^2,$$

so that T^c is a positive operator. Therefore, it has a (Friedrichs) self-adjoint extension T_F^c, a candidate for the energy operator in this situation.

Note that if ψ is in the domain of this Friedrichs extension and it is meaningful to write $u = -\psi'' + c\delta\psi = -\psi'' + c\psi(0)$, then such functions ψ have a slope discontinuity at the origin equal to $c\psi(0)$, so that $u \in \mathrm{L}^2(\mathbb{R})$ even if ψ'' and the constant function $c\psi(0)$ do not.

Exercise 4.4.10. Consider again the formal operator

$$T^c = -\frac{d^2}{dx^2} + c\,\delta(x),$$

as in Example 4.4.9. A possible way to address the problem of getting a well-defined self-adjoint operator is to note that formally on the set

$$E = \{\psi \in \mathcal{H}^2(\mathbb{R}) : \psi(0) = 0\},$$

T^c coincides with $T_0 = -d^2/dx^2$. Show that T_0 with dom $T_0 = E$ is hermitian, that its adjoint has the same action but with dom ${T_0}^* = \{\psi \in \mathcal{H}^2(\mathbb{R} \setminus \{0\}) : \psi(0^-) = \psi(0^+)\}$. Check that its deficiency indices are both equal to 1; the corresponding self-adjoint extensions should contain the rigorous definition of T^c for any $c \in \mathbb{R}$.

Example 4.4.11. The derivative of the Dirac delta $\delta'(x)$ acts formally as

$$\int \delta'(x)\psi(x)dx = -\psi'(x).$$

Here a construction will be discussed so that it becomes meaningful to talk about the energy operator, in $\mathrm{L}^2(\mathbb{R})$,

$$S^c = -\frac{d^2}{dx^2} + c\,\delta'(x), \qquad c < 0.$$

Physically $\delta'(x)$ would model a very strong interaction concentrated at the origin but of positive intensity on the left and of negative intensity on the right, something like a dipole concentrated at the origin (think of the derivative of a function that approximates $\delta(x)$, which has a positive peak on the left and a negative one on the right).

Introduce dom S^c as the set of elements $\psi \in \mathcal{H}^2(\mathbb{R} \setminus \{0\})$ obeying $\psi'(0^+) = \psi'(0^-)$ (both lateral limits do exist), so it becomes meaningful to talk about $\psi'(0) := \psi'(0^+)$ and (a formal integration imposes) $\psi(0^+) - \psi(0^-) = -c\psi'(0)$. This subspace is dense in $\mathrm{L}^2(\mathbb{R})$ since it contains $C_0^\infty(\mathbb{R} \setminus \{0\})$. On dom S^c define the sesquilinear form

$$b_{\delta'}(\psi, \phi) := -\psi'(0)\phi'(0),$$

heuristically corresponding to a δ' potential. Finally, define on dom S^c the operator and subsequent sesquilinear form

$$S^c\psi := -\psi'', \qquad b^{S^c}(\psi, \phi) := \langle \psi, S^c\phi \rangle.$$

On integrating by parts it is found that S^c is hermitian and

$$b^{S^c}(\psi, \phi) = \langle \psi', \phi' \rangle + c\, b_{\delta'}(\psi, \phi),$$

so that

$$b^{S^c}(\psi, \psi) = -c|\psi'(0)|^2 + \|\psi'\|^2$$

and S^c is positive for $c < 0$. Its Friedrichs extension S_F^c is a candidate for the energy operator in this situation. Additional information about δ' potential can be obtained from [Še86] and [ExNZ01].

Exercise 4.4.12. Show that S^c in Example 4.4.11 is hermitian and positive.

Example 4.4.13. Let $\mathcal{H} = \mathrm{L}^2[0,1]$,

$$\begin{aligned}\mathrm{dom}\ T_0 &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = \psi(1) = 0 = \psi'(0) = \psi'(1)\},\\ \mathrm{dom}\ T_1 &= \{\psi \in \mathcal{H}^2[0,1] : \psi(0) = 0 = \psi(1)\},\\ T_j\psi &= -\psi'', \qquad \psi \in \mathrm{dom}\ T_j,\ j = 0,1.\end{aligned}$$

Then $\mathrm{dom}\ T_0^* = \mathcal{H}^2[0,1]$, T_0 is hermitian, lower bounded, with deficiency indices $n_- = n_+ = 2$ (see Example 2.6.8), and the Friedrichs extension of T_0 is $T_F = T_1$. In fact, observe that $T_0 = P^2$, with P as in Example 4.4.3 and $T_1 = P^*P$.

The eigenvectors of T_F form an orthogonal basis of $\mathcal{H}$ and its spectrum is $\{(n\pi)^2 : n = 1,2,3,\dots\}$ (see Example 2.3.5). Then $T_F \geq \pi^2\mathbf{1}$, and the constant π^2 cannot be increased. Check this, for instance, by considering an eigenfunction (of T_F) expansions.

Note, however, that the operator

$$\mathrm{dom}\ T_2 = \left\{\psi \in \mathcal{H}^2[0,1] : \psi(0) = -\psi(1),\ \psi'(0) = -\psi'(1)\right\},$$

$T_2\psi = -\psi''$, is another self-adjoint extension of T_0, with the same spectrum as T_F, and so with the same lower bound π^2. Therefore, the sole lower bound is not enough to characterize the Friedrichs extension of lower bounded hermitian operators.

Exercise 4.4.14. Fill in the missing details in Example 4.4.13.

Exercise 4.4.15. This is closely related to Example 2.3.19. The Hilbert space is $\mathcal{H} = \mathrm{L}^2[0,\infty)$,

$$\mathrm{dom}\ T = \left\{\psi \in \mathcal{H}^2[0,\infty) : \psi(0) = 0,\ \psi'(0) = 0\right\},$$

and $T\psi = -\psi''$.

1. Check that this operator is hermitian and positive.
2. Show that its deficiency indices are $n_- = n_+ = 1$ and that its self-adjoint extensions T_c have the same operator action as T but with domain labeled by $c \in \mathbb{R} \cup \{\infty\}$ with

   $$\mathrm{dom}\ T_c = \left\{\psi \in \mathcal{H}^2[0,\infty) : \psi(0) = c\psi'(0)\right\}, \qquad c \in \mathbb{R},$$

   and $\psi'(0) = 0$ for $c = \infty$.
3. Find the Friedrichs extension T_F of T and conclude that it corresponds to $c = 0$, i.e., the Dirichlet boundary condition is selected.

4.4.1 Hardy's Inequality

An important inequality will be used in the next example. It has versions for $\mathbb{R}^n$, $n > 3$, but with constants different from $1/4$ in Lemma 4.4.16; see Exercise 4.4.21 for $n = 1$.

Lemma 4.4.16 (Hardy's Inequality). *For $\psi \in \mathcal{H}^1(\mathbb{R}^3)$ (in particular for $\psi \in C_0^\infty(\mathbb{R}^3)$)*

$$\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \, dx \geq \frac{1}{4} \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^2} \, dx.$$

Proof. By considering the real and imaginary parts of functions, it is possible to restrict the argument to real-valued ψ. Consider first $\psi \in C_0^\infty(\mathbb{R}^3)$.

For $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ denote $r = |x|$ (standard norm in $\mathbb{R}^3$), and recall that in spherical coordinates (r, θ, φ) one has $dx = r^2 \sin\theta \, dr d\theta d\varphi$. For real-valued $\psi \in C_0^\infty(\mathbb{R}^3)$ set $\phi = r^{\frac{1}{2}}\psi$, so that

$$\begin{aligned} |(\nabla\psi)(x)|^2 &= (\partial_1\psi)^2 + (\partial_2\psi)^2 + (\partial_3\psi)^2 \\ &= \frac{1}{r}|\nabla\phi|^2 - \frac{1}{r^2}\frac{\partial(\phi^2)}{\partial r} + \frac{1}{4r^3}(\phi^2). \end{aligned}$$

Since $\phi(0) = 0$ and there exists $R > 0$ so that $\phi(x) = 0$ if $r \geq R$, then

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{1}{r^2}\frac{\partial(\phi^2)}{\partial r} dx &= \int_0^{2\pi}\int_0^{\pi} \sin\theta \, d\theta d\varphi \int_0^R \frac{\partial(\phi^2)}{\partial r} dr \\ &= \pi \left(\phi(R)^2 - \phi(0)^2\right) = 0. \end{aligned}$$

Therefore

$$\int_{\mathbb{R}^3} |\nabla\psi|^2 \, dx \geq \frac{1}{4}\int_{\mathbb{R}^3} \frac{1}{r^3}\phi^2 \, dx = \frac{1}{4}\int_{\mathbb{R}^3} \frac{1}{r^2}\psi^2 \, dx,$$

which implies the desired inequality in case $\psi \in C_0^\infty(\mathbb{R}^3)$.

For $\psi \in \mathcal{H}^1(\mathbb{R}^3)$, take a sequence $(\psi_j)_j \subset C_0^\infty(\mathbb{R}^3)$ with $\psi_j \to \psi$ in $\mathcal{H}^1(\mathbb{R}^3)$; thus both $\psi_j \to \psi$ and (the components of) $\nabla\psi_j \to \nabla\psi$ in $\mathrm{L}^2(\mathbb{R}^3)$, and the inequality follows for all $\psi \in \mathcal{H}^1(\mathbb{R}^3)$. □

Exercise 4.4.17. Inspect the proof of Hardy's inequality to show that equality holds for $\psi \in C_0^\infty(\mathbb{R}^3)$ iff $\psi = 0$.

Remark 4.4.18. There is a version of Hardy's inequality in $\mathbb{R}^n$, $n \geq 3$, that holds for all $\psi \in \mathcal{H}^1(\mathbb{R}^n)$ and takes the form

$$\int_{\mathbb{R}^n} |\nabla\psi(x)|^2 \, dx \geq \frac{(n-2)^2}{4} \int_{\mathbb{R}^n} \frac{|\psi(x)|^2}{|x|^2} \, dx,$$

and the constant $(n-2)^2/4$ is the best possible for all $\psi \in C_0^\infty(\mathbb{R}^n)$ [Sh31], [KaSW75].

Example 4.4.19. [The Friedrichs Extension for the 3D hydrogen atom] Let $\mathcal{H} = \mathrm{L}^2(\mathbb{R}^3)$ and consider $\operatorname{dom} H = C_0^\infty(\mathbb{R}^3)$ and

$$(H\psi)(x) = -\frac{\hbar^2}{2m}(\Delta\psi)(x) - \alpha\frac{e^2}{|x|}\psi(x), \qquad \psi \in \operatorname{dom} H,$$

with $\alpha > 0$. This is related to the quantum three-dimensional (briefly 3D) hydrogen atom energy operator (with some physical constants included: Planck constant $\hbar$, electron mass m and charge $-e$). Integration by parts shows that H is hermitian and, together with Lemma 4.4.16 that, for real-valued $\psi \in \operatorname{dom} H$,

$$\begin{aligned}\langle\psi, H\psi\rangle &= \int_{\mathbb{R}^3}\left(\frac{\hbar^2}{2m}|\nabla\psi(x)|^2 - \alpha\frac{e^2}{|x|}\psi(x)^2\right)dx \\ &\geq \int_{\mathbb{R}^3}\left(\frac{\hbar^2}{8m}\frac{1}{|x|^2} - \alpha\frac{e^2}{|x|}\right)\psi(x)^2\,dx.\end{aligned}$$

Now pick $a > 0$ so that

$$\frac{\alpha e^2}{|x|} \leq \frac{\hbar^2}{8m|x|^2} + a, \qquad \forall x \neq 0.$$

Thus

$$\langle\psi, H\psi\rangle \geq -a\int_{\mathbb{R}^3}\psi(x)^2\,dx = -a\|\psi\|^2.$$

For $\psi = \psi_1 + i\psi_2 \in \operatorname{dom} H$, with ψ_1, ψ_2 real-valued, one gets

$$\begin{aligned}\langle\psi, H\psi\rangle &= \langle\psi_1, H\psi_1\rangle + i\langle\psi_1, H\psi_2\rangle - i\langle\psi_2, H\psi_1\rangle + \langle\psi_2, H\psi_2\rangle \\ &= \langle\psi_1, H\psi_1\rangle + \langle\psi_2, H\psi_2\rangle \\ &\geq -a\|\psi_1\|^2 - a\|\psi_2\|^2 = -a\|\psi\|^2,\end{aligned}$$

and the same relation holds for all elements of $\operatorname{dom} H$. Therefore, it follows that $H \geq -a\mathbf{1}$ and H has the self-adjoint Friedrichs extension H_F. Further, $H_F \geq -a\mathbf{1}$ and its spectrum $\sigma(T_F)$ is lower bounded.

Remark 4.4.20. By using results of Rellich, in the 1950s Tosio Kato showed that H in Example 4.4.19 with domain $C_0^\infty(\mathbb{R}^3)$ is essentially self-adjoint; this is discussed in Example 6.2.3.

Exercise 4.4.21. Let ψ be a real-valued element of $C_0^\infty(\mathbb{R}\setminus\{0\})$ or $C_0^\infty(0,\infty)$. On integrating by parts

$$\int \psi(x)^2\frac{1}{x^2}\,dx,$$

and then applying Cauchy-Schwarz, conclude the Hardy's inequality

$$\frac{1}{4}\int\left(\frac{\psi(x)}{x}\right)^2 dx \leq \int \psi'(x)^2\,dx.$$

The integrations are over $\mathbb{R}$ or $[0,\infty)$, respectively.