Self-adjoint extensions of symmetric operators

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Abstract

In this handout we will first look at some basics about unbounded operators. Those will be used to give the definition of self-adjoint operators and self-adjoint extension of an operator. Furthermore, a brief introduction to the basics of quantum mechanics will give some motivations to derive criteria for self-adjointness and for the existence of self-adjoint extensions of symmetric operators.

Contents

1 Motivations: Why do we need self-adjoint operators in physics?

In this handout we will look at some definitions and basic properties of unbounded operators. It is natural to ask why we need all of this mathematical machinery. Surely it is an interesting mathematical topic by itself, but its use goes far beyond pure mathematical interest. In physics, especially quantum mechanics, self-adjoint operators play a crucial role. They do not only describe a physical system, but one can actually draw a connection between the pure mathematical concept and the actual measurements in a physical system.

To illustrate this connection we should first recall that in quantum mechanics a physical system is described by operators on a separable Hilbert space $\mathcal{H}$ and the vectors of norm one describe a physical state. Two vectors correspond to the same state if they only differ by a complex factor of absolute value one, a so-called phase factor. The behaviour of the system is described by operators on $\mathcal{H}$.

In an experiment, what we basically do is measuring the eigenvalues of operators. Now one can easily imagine that it is not possible to measure a complex value of some sort. Therefore, one of the basic assumptions in quantum dynamics is that every operator that corresponds to a physical observable has to have real eigenvalues. We will see in the next section that for an operator this assumption is equivalent to its self-adjointness.

The so-called Hamilton operator, whose eigenvalues correspond to the energy of a system, is of special interest, since it is used to calculate the dynamic behaviour of a physical system. One fundamental equation involving this operator is the Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}[U(t)\varphi] = iH[U(t)\varphi],$$

where H is the Hamilton operator and $U(t)$ is the so-called time evolution operator. It describes the dynamic behaviour of a system, i.e. if the system is in the state φ at a time $t_0 = 0$, then it is in the state $U(t)\varphi$ at the time t. The operator $U(t)$ is determined by the Hamilton operator H and to show the existence of $U(t)$ the self-adjointness of H is needed.

It is usually quite simple to come up with a formal expression for the Hamiltonian associated to a system by using physical reasonings. But since physicists are "pretty lazy" they usually do not really think about domains but just start calculating and afterwards say "the domain is where this works". Of course this will not always work and one of the essential mathematical problems is to exactly determine the domain of a formal operator, and whether or not it is symmetric, self-adjoint, etc. and, when necessary, find the appropriate extension with such properties.

In Section 2 we will introduce notations and basic definitions, which will be used in Section 3 to state and prove criteria for the self-adjointness and the existence of self-adjoint extensions of unbounded linear operators. Section 4 will be devoted to an explicit physical example where we use the results presented in the former sections.

2 Preliminaries on bounded and unbounded operators

Before introducing symmetric and self-adjoint operators and their meaning in physics, we will revise some basic definitions.

Definition 2.1 (Bounded and unbounded linear operators)**.** Let $T : \mathcal{H}_1 \to \mathcal{H}_2$ be a linear operator between normed vector spaces. Then T is called **bounded** if

$$\exists M > 0 : \forall x \in \mathcal{H}_1 : \|Tx\|_{\mathcal{H}_2} \leq M\|x\|_{\mathcal{H}_1},$$

otherwise T is called **unbounded**.

Equivalently, one can define the **operator norm** by

$$\|T\| = \sup_{x \in \mathcal{H}_1, x \neq 0} \frac{\|Tx\|_{\mathcal{H}_2}}{\|x\|_{\mathcal{H}_1}}$$

and say that T is bounded if $\|T\| < \infty$.

Note that any linear operator between finite-dimensional normed spaces is bounded (this easily follows from the equivalence of all norms on a finite-dimensional vector space). The matrix norm is then equivalent to the operator norm and thus the operator is bounded. In the following let $\mathcal{H}$ be a Hilbert space, i.e. an inner product space which is also complete with respect to the topology given by the metric induced by its scalar product $\langle \cdot, \cdot \rangle$. The Hellinger-Toeplitz theorem [1, p.84] states that any everywhere-defined operator T on $\mathcal{H}$ satisfying $\forall x, y \in \mathcal{H} : \langle Tx, y \rangle = \langle x, Ty \rangle$ is necessarily bounded. This suggests that an unbounded operator which is not self-adjoint is not defined everywhere. Therefore, whenever talking about an unbounded operator on $\mathcal{H}$ we mean a linear map from a **domain** into $\mathcal{H}$. The domain of T will be denoted by $D(T)$ and in this handout is assumed to be a linear subspace of $\mathcal{H}$.

To define a general unbounded operator T we must always give its domain $D(T)$ alongside the formal definition. Keep this slogan in mind:

Unbounded operator = *Domain* + *how it acts*

Before giving an example for an unbounded operator we will get familiar with the probably most common vector space in physics: $L^2(\mathbb{R})$.

Example 2.2. The space $L^2(\mathbb{R})$ consists of all the equivalence classes of almost everywhere equal real functions satisfying $\int_{\mathbb{R}} |f(x)|^2 \mathrm{d}x < \infty$. A scalar product on $L^2(\mathbb{R})$ is given by

$$\langle f, g \rangle = \int_{\mathbb{R}} f(x) g(x) \mathrm{d}x \quad \text{for all} \quad f, g \in L^2(\mathbb{R}),$$

inducing the norm

$$\|f\|^2 = \langle f, f \rangle = \int_{\mathbb{R}} f(x)^2 \mathrm{d}x \quad \text{for all} \quad f \in L^2(\mathbb{R}).$$

This vector space is commonly used in quantum mechanics. Physical arguments give a function in $L^2(\mathbb{R})$ that represents a special state of a physical system that might for example correspond to a particle. This gets a bit clearer in the next example.

Example 2.3 (Position operator)**.** Let $D(T) \subseteq L^2(\mathbb{R})$ be the set of all functions $\varphi \in L^2(\mathbb{R})$ satisfying $\int_{\mathbb{R}} x^2|\varphi(x)|^2 dx < \infty$. We define the position operator T by $(T\varphi)(x) := x\varphi(x)$, $\forall \varphi \in D(T)$, $\forall x \in \mathbb{R}$. T is called the position operator since if φ represents a quantum mechanical particle, then $\|T\varphi\|$ corresponds to its position. It is straight forward to see the unboundedness of this operator. Indeed, if we choose the function φ to have support near infinity whilst keeping $\|\varphi\| = 1$, we can increase $\|T\varphi\|$ arbitrarily, e.g. we can take φ to be a rectangular function or a Gaussian function with support near to $+\infty$. While both example functions can be normalized to $\|\varphi\| = 1$, $\|T\varphi\|$ will correspond to the "position of the peak" and so if the peak is close to plus or minus infinity we have the desired behaviour, i.e. $\|T\| = \infty$. To illustrate this we will explicitly calculate the norms for a Gaussian function $\varphi(x) = \frac{\mathrm{e}^{-\frac{1}{2}(x-t)^2}}{\sqrt[4]{\pi}}$ for some $t \in \mathbb{R}$. Remembering the standard Gaussian integral one gets:

$$\|\varphi\|^2 = \int_{-\infty}^{\infty} \left(\frac{\mathrm{e}^{-\frac{1}{2}(x-t)^2}}{\sqrt[4]{\pi}} \right)^2 \mathrm{d}x = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-(x-t)^2} \mathrm{d}x = \frac{1}{\sqrt{\pi}} \sqrt{\pi} = 1.$$

On the other hand

$$\|T\varphi\|^2 = \int_{-\infty}^{\infty} \left(x \frac{\mathrm{e}^{-\frac{1}{2}(x-t)^2}}{\sqrt[4]{\pi}} \right)^2 \mathrm{d}x = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} x^2 \mathrm{e}^{-(x-t)^2} \mathrm{d}x = t^2 + \frac{1}{2},$$

where the last integral can for example be calculated using the momentum generating function of the standard normal distribution known from stochastics. Here we can see that we are free to choose t without altering $\|\varphi\|$, but we can choose t for $\|T\varphi\|$ to be arbitrarily large.

Note, that in general even if $\varphi \notin D(T)$, $T\varphi$ might still be a well defined function but not contained in $L^2(\mathbb{R})$. Hence, to remain in $L^2(\mathbb{R})$ we need to restrict the domain of T in the above manner.

The next definitions are very important for the study of unbounded operators.

Definition 2.4 (Graph and closed operator)**.** The **graph** of a linear transformation T with domain $D(T) \subseteq \mathcal{H}$ is the set

$$\Gamma(T) = \{(\varphi, T\varphi) \mid \varphi \in D(T)\}.$$

T is called **closed** if $\Gamma(T)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$ endowed with the product topology.

Using these two notions, one can now define extensions and closability of linear operators.

Definition 2.5 (Extension and closable operators)**.**
(i) Let T_1 and T be linear operators on $\mathcal{H}$. T_1 is called an **extension** of T if $\Gamma(T) \subset \Gamma(T_1)$. We write $T \subset T_1$. An equivalent definition is $T \subset T_1$ if and only if $D(T) \subset D(T_1)$ and $T_1\varphi = T\varphi$ for all $\varphi \in D(T)$.

(ii) An operator T is **closable** if it has a closed extension. The smallest closed extension (w.r.t. "$\subset$") is called its **closure** and is denoted by $\overline{T}$.

We are now ready to give one of the central definitions in this section, which we are going to use extensively in the rest of this handout.

Definition 2.6 (Adjoint)**.** Let T be a densely defined linear operator on $\mathcal{H}$ (i.e. $D(T)$ is dense in $\mathcal{H}$) and $D(T^*)$ be the subset of $\mathcal{H}$ containing all the $\varphi \in \mathcal{H}$, such that there is a $\eta \in \mathcal{H}$ satisfying

$$\langle T\psi, \varphi\rangle = \langle \psi, \eta\rangle \quad \text{for all} \quad \psi \in D(T). \tag{1}$$

For all such $\varphi \in D(T^*)$ the **adjoint** operator T^* is defined by $T^*\varphi = \eta$. Note that by the Riesz representation theorem [1, Thm.11.4, p. 43] [1], $\varphi \in D(T^*)$ if and only if $|\langle T\psi, \varphi\rangle| \leq C\|\psi\|_{\mathcal{H}}$ for some $C > 0$. Note also that η is uniquely determined in (1) because of the density of $D(T)$ in $\mathcal{H}$.

Let us now look at some basic properties of the adjoint operator.

Theorem 2.7. *Let T be a densely defined operator on $\mathcal{H}$. Then:*

(i) T^* is closed.

(ii) T is closable if and only if $D(T^*)$ is dense in which case $\overline{T} = T^{**}$.

(iii) If T is closable, then $(\overline{T})^* = T^*$.

Proof. [1, Thm.VIII.1, p.252-253]. □

An important tool for characterizing closed operators is the resolvent set.

Definition 2.8 (Resolvent set)**.** Let T be a closed operator on $\mathcal{H}$. A complex number λ is in the **resolvent set** $\rho(T)$, if $\lambda I - T$ is a bijection of $D(T)$ onto $\mathcal{H}$ with a bounded inverse. If $\lambda \in \rho(T)$, $R_\lambda(T) := (\lambda I - T)^{-1}$ is called the **resolvent** of T at λ.

Remark 2.9. In this definition the conditions are not all independent. In fact, using the closed graph theorem [1, Thm.III.12, p.83] one can show that if $\lambda I - T$ is a bijection of $D(T)$ onto $\mathcal{H}$, then the inverse is automatically bounded.

The definition of spectrum for unbounded operators is the same as in the bounded case:

Definition 2.10 (Spectrum)**.** Let T be a linear operator in $\mathcal{H}$.

[1] Here we are using a more general version than the one known from Linear Algebra I/II. This version also applies to infinite dimensional Hilbert spaces.

(i) If $\lambda \in \mathbb{C}$ is not in the resolvent set ($\lambda \notin \rho(T)$), then λ is said to be in the **spectrum** $\sigma(T)$ of T.

(ii) An $0 \neq x \in \mathcal{H}$ that satisfies $Tx = \lambda x$ for some $\lambda \in \mathbb{C}$ is called an **eigenvector** of T; λ is called the corresponding **eigenvalue**. If λ is an eigenvalue of T, then $\lambda I - T$ is not injective and $\lambda \in \sigma(T)$. The set of all eigenvalues of T is called the **point spectrum** of T.

(iii) If λ is not an eigenvalue and if $\mathrm{Ran}(\lambda I - T)$ is not dense, then λ is said to be in the **residual spectrum**.

Remark 2.11. One can show that the resolvent set is an open subset of the complex plane (see [1, Thm.VIII.2, p. 254]) and thus the spectrum is a closed subset of the complex plane.

The spectrum is one of the most important characteristics of an operator and is of great interest, especially in physics, as it was illustrated in Section 1. We are now ready to make an example about the great influence of the domain on the structure of the spectrum of an unbounded operator.

Example 2.12 (Domain makes huge difference)**.** Consider the set $AC[0,1]$ of absolutely continuous functions[2] on $[0,1]$ whose first derivatives are in $L^2[0,1]$. Let T_1 and T_2 be the operator $i\frac{\mathrm{d}}{\mathrm{d}x}$ with the domains

$$D(T_1) = \{\varphi \in L^2[0,1] \mid \varphi \in AC[0,1]\},$$
$$D(T_2) = \{\varphi \in L^2[0,1] \mid \varphi \in AC[0,1] \quad \text{and} \quad \varphi(0) = 0\}.$$

Both $D(T_1)$ and $D(T_2)$ are dense in $L^2[0,1]$ and both operators are closed, but

$$\sigma(T_1) = \mathbb{C} \neq \emptyset = \sigma(T_2). \tag{2}$$

Let us just show (2).

(i) Note that $\mathrm{e}^{-i\lambda x} \in D(T_1)$ and $(\lambda I - T_1)\mathrm{e}^{-i\lambda x} = \lambda \mathrm{e}^{-i\lambda x} - i\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-i\lambda x} = \lambda \mathrm{e}^{-i\lambda x} - \lambda \mathrm{e}^{-i\lambda x} = 0$ for every $\lambda \in \mathbb{C}$. Therefore, any $\lambda \in \mathbb{C}$ is an eigenvalue and so $\sigma(T_1) = \mathbb{C}$.

(ii) For determining $\sigma(T_2)$, let us look at the operator S_λ defined by

$$(S_\lambda g)(x) = i\int_0^x \mathrm{e}^{-i\lambda(x-s)} g(s)\mathrm{d}s \quad \forall g \in D(T_2), \forall \lambda \in \mathbb{C}.$$

[2] f is called absolutely continuous on $[a,b]$ if f has a derivative f' almost everywhere, the derivative is Lebesgue integrable, and $f(x) = f(a) + \int_a^x f'(t)\mathrm{d}t$ for all x on $[a,b]$.

For any $\lambda \in \mathbb{C}$ we have $(\lambda I - T_2)S_\lambda = I = S_\lambda(\lambda I - T_2)$ on $D(T_2)$. Indeed, let $g \in D(T_2)$, then

$$\begin{aligned}
(\lambda I - T_2)S_\lambda g(x) &= \lambda S_\lambda g(x) - i\frac{\mathrm{d}}{\mathrm{d}x} i \int_0^x \mathrm{e}^{-i\lambda(x-s)} g(s)\mathrm{d}s \\
&= \lambda S_\lambda g(x) + \frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-i\lambda x} \int_0^x \mathrm{e}^{i\lambda s} g(s)\mathrm{d}s \\
&= \lambda S_\lambda g(x) - i\lambda \mathrm{e}^{-i\lambda x} \int_0^x \mathrm{e}^{i\lambda s} g(s)\mathrm{d}s + \mathrm{e}^{-i\lambda x}\mathrm{e}^{i\lambda x} g(x) \\
&= \lambda S_\lambda g(x) - \lambda S_\lambda g(x) + g(x) = g(x),
\end{aligned}$$

and

$$\begin{aligned}
S_\lambda(\lambda I - T_2)g(x) &= \lambda S_\lambda g(x) - iS_\lambda g'(x) = \lambda S_\lambda g(x) - i^2 \int_0^x \mathrm{e}^{-i\lambda(x-s)} g'(s)\mathrm{d}s \\
&= \lambda S_\lambda g(x) + [\mathrm{e}^{-i\lambda(x-s)} g(s)]_0^x - i \int_0^x \lambda \mathrm{e}^{-i\lambda(x-s)} g(s)\mathrm{d}s \\
&= \lambda S_\lambda g(x) + \underbrace{\mathrm{e}^{-i\lambda(x-x)}}_{=1} g(x) - \mathrm{e}^{-i\lambda x} \underbrace{g(0)}_{=0} - \lambda S_\lambda g(x) \\
&= g(x).
\end{aligned}$$

Therefore, we found the inverse of $(\lambda I - T_2)$ on $D(T_2)$, which is therefore bijective. Because of Remark 2.9 we do not need to prove the boundedness of S_λ and thus for any $\lambda \in \mathbb{C}$ we have $\lambda \in \rho(T_2)$ and $\lambda \notin \sigma(T_2)$, i.e. $\sigma(T_2) = \emptyset$.

We will now introduce another basic definition for this topic.

Definition 2.13. Let T be a densely defined operator on a Hilbert space $\mathcal{H}$.

(i) T is called **symmetric** (or **hermitian**) if $T \subset T^*$, i.e. $D(T) \subset D(T^*)$, and $T\varphi = T^*\varphi$ for all $\varphi \in D(T)$. Equivalently, T is symmetric if and only if

$$\langle T\varphi, \psi \rangle = \langle \varphi, T^*\psi \rangle \quad \text{for all} \quad \varphi, \psi \in D(T).$$

(ii) T is called **self-adjoint** if $T = T^*$, that is, if and only if T is symmetric and $D(T) = D(T^*)$.

(iii) T is called **essentially self-adjoint** if its closure $\overline{T}$ is self-adjoint.

Remark 2.14. Note that since a symmetric operator T is densely defined and $D(T^*) \supset D(T)$, we have that $D(T^*)$ is dense in $\mathcal{H}$. Then by Theorem 2.7(ii) we have that T is closable. This means that any symmetric operator is always closable. For a symmetric T, the adjoint T^* is a closed extension and the smallest closed extension T^{**} of T (see Theorem 2.7(ii)) must be contained in T^*. Thus for symmetric operators the relation

$$T \subset T^{**} \subset T^*$$

holds, while for closed symmetric operators we get

$$T = T^{**} \subset T^*.$$

For self-adjoint operators this relation reads

$$T = T^{**} = T^*.$$

From this, one can easily see that a closed symmetric operator T is self-adjoint if and only if T^* is symmetric.

3 Criteria for the existence of self-adjoint extensions

In this section we focus on some criteria for establishing the self-adjointness of an operator and the existence of self-adjoint extensions. An important tool for that is the spectrum (see Definition 2.10).

Theorem 3.1. *Let T be a closed symmetric operator on a Hilbert space $\mathcal{H}$. Then*

(i) $\dim[\mathrm{Ker}(\lambda I - T^*)]$ *is constant throughout the open upper half-plane.*

(ii) $\dim[\mathrm{Ker}(\lambda I - T^*)]$ *is constant throughout the open lower half-plane.*

*(iii) The spectrum of T is **one** of the following:*

- *a) the closed upper half-plane,*
- *b) the closed lower half-plane,*
- *c) the entire plane,*
- *d) a subset of the real axis.*

*(iv) T is self-adjoint if and only if the dimensions in both (ii) **and** (i) are zero.*

(v) T is self-adjoint if and only if case (iii-d) holds.

Proof. (i,ii): Let $\lambda \in \mathbb{C}\backslash\mathbb{R}$, i.e. $\mathrm{Im}\lambda \neq 0$. Using the symmetry of T we get

$$\begin{aligned} \|(\lambda - T)\varphi\|^2 &= \langle(\mathrm{Re}\lambda - T)\varphi, (\mathrm{Re}\lambda - T)\varphi\rangle + \langle \mathrm{Im}\lambda\varphi, \mathrm{Im}\lambda\varphi\rangle \\ &\quad + \underbrace{\langle \mathrm{Im}\lambda\varphi, (\mathrm{Re}\lambda - T)\varphi\rangle + \langle(\mathrm{Re}\lambda - T)\varphi, \mathrm{Im}\lambda\varphi\rangle}_{=0} \\ &= \|(\mathrm{Re}\lambda - T)\varphi\|^2 + |\mathrm{Im}\lambda|^2\|\varphi\|^2 \geq |\mathrm{Im}\lambda|^2\|\varphi\|^2 \end{aligned} \tag{3}$$

for all $\varphi \in D(T)$. To show that $\mathrm{Ran}(\lambda - T)$ is closed, let us consider a sequence $(\varphi_m)_{n\in\mathbb{N}} \subset D(T)$, $\varphi_m \to \varphi_0$ such that $(\lambda - T)\varphi_m \to \psi$. Since T is closed we know $T\varphi_m \to T\varphi_0$ and $\varphi_0 \in D(T)$, $T\varphi_0$ in $\mathrm{Ran}(T)$. Thus $\psi = \lambda\varphi_0 - T\varphi_0 = (\lambda - T)\varphi_0$, i.e. $\psi \in \mathrm{Ran}(\lambda - T)$ and $\mathrm{Ran}(\lambda - T)$ is a closed subset of $\mathcal{H}$. Furthermore, let $\varphi \in D(T^*)$, then

$$\varphi \in \mathrm{Ker}(\lambda - T^*) \Leftrightarrow 0 = \langle(\lambda - T^*)\varphi, \varphi\rangle = \langle\varphi, (\overline{\lambda} - T)\varphi\rangle \Leftrightarrow \varphi \in \mathrm{Ran}(\overline{\lambda} - T)^\perp. \tag{4}$$

Using (4) one can show that for any $\lambda \in \mathbb{C}\backslash\mathbb{R}$ there exists a neighbourhood U_λ with $U_\lambda \cap \mathbb{R} = \emptyset$ (i.e. the neighbourhood is completely contained in the same half-plane as λ) such that for any $\tilde{\lambda} \in U_\lambda$ we have $\dim \operatorname{Ker}(\tilde{\lambda} - T) = \dim \operatorname{Ker}(\lambda - T)$. This means that the dimension is constant throughout each of the two open half-planes. Note that the constant $\dim \operatorname{Ker}(\lambda - T)$ can be different for the upper and lower half-plane.

(iii): Since from (3) we get $\|(\lambda - T)^{-1}\| = \|(\lambda - T)\|^{-1} \leq |\mathrm{Im}\lambda|^{-1}$ we know that $\lambda - T$ has a bounded inverse if $\mathrm{Im}\lambda \neq 0$. From (4) we find, that the inverse is defined everywhere if and only if $\operatorname{Ran}(\lambda - T)^\perp = \operatorname{Ker}(\overline{\lambda} - T) = \{0\}$, i.e. $\dim \operatorname{Ker}(\overline{\lambda} - T) = 0$. From (ii,i) it follows, that each of the half-planes is either completely in the resolvent (i.e. $(\lambda - T)$ has an everywhere defined, bounded inverse) or in the spectrum. Since we know from Remark 2.11 that the spectrum is closed, we can construct all the cases in (iii).

(iv): " $\Rightarrow$ ": Let T be self-adjoint and assume there is $\lambda \in \mathbb{C}\backslash\mathbb{R}$ such that $\lambda \in \sigma(T)$. Then there is $0 \neq \varphi \in D(T^*) = D(T)$ such, that $T\varphi = \lambda = T^*\varphi$ and we can compute

$$\lambda \langle \varphi, \varphi \rangle = \langle \lambda\varphi, \varphi \rangle = \langle T\varphi, \varphi \rangle = \langle \varphi, T^*\varphi \rangle = \langle \varphi, \lambda\varphi \rangle = \overline{\lambda} \langle \varphi, \varphi \rangle .$$

Thus we see that $2\mathrm{Im}\lambda \langle \varphi, \varphi \rangle = 0$, i.e. $\varphi = 0$ for $\mathrm{Im}\lambda \neq 0$. Therefore, $\lambda \notin \sigma(T)$ and $\operatorname{Ker}(\lambda - T^*) = \{0\}$ and $\dim \operatorname{Ker}(\lambda - T^*) = 0$. This holds regardless the sign of $\mathrm{Im}\lambda$ and therefore this direction is proven.

" $\Leftarrow$ ": Assume $\dim \operatorname{Ker}(\lambda - T^*) = 0$ for all $\lambda \in \mathbb{C}\backslash\mathbb{R}$. Then also $\dim \operatorname{Ker}(\overline{\lambda} - T^*) = 0$for all $\lambda \in \mathbb{C}\backslash\mathbb{R}$ and using (4) we get $\operatorname{Ran}(\lambda - T) = \mathcal{H}$ for case (ii). Let $\varphi \in D(T^*)$, then there exists a $\eta \in D(T)$ such, that $(\lambda - T)\eta = (\lambda - T^*)\varphi$. Since $D(T) \subset D(T^*)$ we get $\varphi - \eta \in D(T^*)$ and

$$(\lambda - T^*)(\varphi - \eta) = (\lambda - T^*)\varphi - (\lambda - T^*)\eta = (\lambda - T)\eta - (\lambda - T^*)\eta = \underbrace{(T^* - T)}_{=0,\text{ since } T \text{ sym.}} \eta = 0.$$

Since $\operatorname{Ker}(\lambda - T^*) = \{0\}$ we get $\varphi = \eta \in D(T)$, i.e. $D(T) = D(T^*)$ and T is self-adjoint.

(v) Case (iii-d) is equivalent to $\lambda \in \rho(T)$ for all $\lambda \in \mathbb{C}\backslash\mathbb{R}$, i.e. $\operatorname{Ran}(\lambda - T) = \mathcal{H}$. Using (4) we see that $\operatorname{Ker}(\overline{\lambda} - T^*) = \operatorname{Ran}(\lambda - T)^\perp = \{0\}$ and thus by (iv) this is equivalent to the self-adjointness of T. □

Note that Theorem 3.1(iv) leads to a very basic criterion for self-adjointness:

Corollary 3.2. *Let T be a closed symmetric operator on $\mathcal{H}$. T is self-adjoint if and only if* $\operatorname{Ker}(T^* \pm i) = \{0\}$.

Furthermore Theorem 3.1(v) gives a very easy criterion:

Corollary 3.3. *If a closed symmetric operator T has at least one real number in its resolvent set, i.e. $\rho(T) \cap \mathbb{R} \neq \emptyset$, then it is self-adjoint.*

We now introduce a way to give explicit self-adjoint extensions.

Definition 3.4 (deficiency subspaces and deficiency indices)**.** Suppose T is a symmetric operator. Let

$$\mathcal{K}_+ = \operatorname{Ker}(i - T^*) = \operatorname{Ran}(i + T)^\perp$$
$$\mathcal{K}_- = \operatorname{Ker}(i + T^*) = \operatorname{Ran}(-i + T)^\perp$$

$\mathcal{K}_+$ and $\mathcal{K}_-$ are called the **deficiency subspaces** of T. The pair of numbers n_+, n_- given by $n_+(T) = \dim(\mathcal{K}_+)$, $n_-(T) = \dim(\mathcal{K}_-)$ are called the **deficiency indices** of T.

Note that (n_+, n_-) can take any value in $(\mathbb{N}_0 \cup \{\infty\}) \times (\mathbb{N}_0 \cup \{\infty\})$.

Theorem 3.5. *Let T be a closed symmetric operator. The closed symmetric extensions of T are in one-to-one correspondence with the set of partial isometries (in the usual inner product) of $\mathcal{K}_+$ into $\mathcal{K}_-$. If U is such an isometry with domain $I(U) \subseteq \mathcal{K}_+$, then the corresponding closed symmetric extension T_U has domain*

$$D(T_U) = \{\varphi + \varphi_+ + U\varphi_+ \mid \varphi \in D(T), \varphi_+ \in I(U)\}$$

and

$$T_U(\varphi + \varphi_+ + U\varphi_+) = T\varphi + i\varphi_+ - iU\varphi_+.$$

If $\dim I(U) < \infty$, the deficiency indices of T_U are

$$n_\pm(T_U) = n_\pm(T) - \dim I(U).$$

Proof. [2, Thm.X.2, p.140]. □

Corollary 3.6. *Let T be a closed symmetric operator with deficiency indices $n_\pm$. Then*

(i) T is self-adjoint if and only if $n_+(T) = 0 = n_-(T)$.

(ii) T has self-adjoint extensions if and only if $n_+(T) = n_-(T)$. There is a one-to-one correspondence between self-adjoint extensions of T and unitary maps from $\mathcal{K}_+$ onto $\mathcal{K}_-$.

*(iii) If either $n_+(T) = 0 \neq n_-(T)$ or $n_-(T) = 0 \neq n_+(T)$, then T has no nontrivial symmetric extensions (such operators are called **maximal symmetric**).*

4 Physical example: Schroedinger particle on a half-line

Let $(T\varphi)(x) := -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\varphi(x)$ in $L^2(0,\infty)$ with domain $C_0^\infty(0,\infty)$, where $C_0^\infty(0,\infty)$ is the space of all infinitely continuous differentiable functions that tend to zero for $x \to 0, \infty$. To determine the deficiency indices (see Definition 3.4) we look at $\operatorname{Ker}(i \pm T^*)$ and so we look at $T^*\varphi = \pm i\varphi$. Using the theory of differential equations, we can find the infinitely differentiable solutions

$$\psi_\pm(x) = \mathrm{e}^{\frac{\pm(-1+i)x}{\sqrt{2}}} \quad \text{to} \quad T^*\varphi = +i\varphi \quad \text{and}$$
$$\chi_\pm(x) = \mathrm{e}^{\frac{\pm(1+i)x}{\sqrt{2}}} \quad \text{to} \quad T^*\varphi = -i\varphi.$$

Looking at the sign of the real part in the exponential and recalling the Gaussian integral we see that $\psi_-, \chi_+ \notin L^2(0,\infty)$. Thus we find the deficiency indices of T to be $(1,1)$. We now want to use Theorem 3.5 to determine explicitly the self-adjoint extensions of T. So we are looking for isometries that map a multiple of $\tilde{\psi} = \psi_+/\|\psi_+\| = \sqrt{2}\mathrm{e}^{\frac{(-1+i)x}{\sqrt{2}}}$ onto a multiple of $\tilde{\chi} = \chi_-/\|\chi_-\| = \sqrt{2}\mathrm{e}^{\frac{-(1+x)}{\sqrt{2}}}$. Since $\tilde{\psi}$ and $\tilde{\chi}$ are normalized the only possible isometries are maps $\tilde{\psi} \to \gamma\tilde{\chi}$ where $|\gamma| = 1$. We therefore get that the corresponding self-adjoint extensions are all $\{T_\gamma \mid \gamma \in \mathbb{C}, |\gamma| = 1\}$ with:

$$D(T_\gamma) = \{\varphi + \beta\tilde{\psi} + \beta\gamma\tilde{\chi} \mid \varphi \in C_0^\infty, \beta \in \mathbb{C}\}.$$

One can simplify this domain in a clever way. Let $f \in D(T_\gamma)$. By calculating $f(0)$ and $f'(0)$ we can show that either $\exists\alpha \in \mathbb{R}$ such that $f'(0) + \alpha f(0) = 0$ (where α only depends on γ) or $f(0) = 0$. The latter case corresponds to $\alpha = \infty$, which is equivalent to $\gamma = -1$. We can also show, that $f \in AC^2[0,\infty] := \{g \in AC[0,\infty] \mid g \text{ is continousely differentiable}\}$ and so the domains can be written as

$$D(T_\alpha) = \{f \mid f \in AC^2[0,\infty], f'(0) + \alpha f(0) = 0\}$$
$$D(T_\infty) = \{f \mid f \in AC^2[0,\infty], f(0) = 0\}.$$

Now let us do some physical interpretation. Since the momentum operator (similar to the position operator) is given by $-i\frac{\mathrm{d}}{\mathrm{d}x}$ and $-i\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-ikx} = -k\mathrm{e}^{-ikx}$, the function e^{-ikx} represents a plane wave moving to the left with momentum $k > 0$. The same argument leads to the interpretation of e^{ikx} as a wave moving right with momentum k. Of course both e^{-ikx} and e^{ikx} are not in $L^2(0,\infty)$ but, since we are "lazy physicists", for now we are only interested in the behaviour near zero and so we can ignore that. Both functions are not in $D(T_\alpha)$ as they do not satisfy the boundary conditions for a fixed $\alpha > 0$. On the other hand, defining $a = \frac{ik-\alpha}{ik+\alpha}$ the function $f(x) = \mathrm{e}^{-ikx} + a\mathrm{e}^{ikx}$ satisfies $f'(0) + \alpha f(0) = 0$ and thus $f \in D(T_\alpha)$ (ignoring the behaviour at ∞).

Physically speaking f is a superposition of an incoming wave and a phase shifted outgoing wave. Thus the physical interpretation of the boundary condition is that an incoming wave gets reflected at the origin with a phase change of $a(k) = \frac{ik-\alpha}{ik+\alpha}$. The case $\alpha = \infty$ corresponds to a so-called "hard wall potential" that results in a phase change of $a = -1$ for all momenta.

Since the phase change is different for the different self-adjoint extensions, they all correspond to different physical systems, that might have completely distinct properties.

References

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