11. UNBOUNDED OPERATORS AND RELATIONS

Many important operators on Hilbert spaces are not bounded. For example, differential operators on $L^2(\mathbb{R}^n)$ are never bounded. Therefore, we now want to analyze general linear operators T on H, not necessarily bounded or, equivalently, continuous. We also drop the assumption that T is defined on all of H, so we now consider operators $T: D(T) \to H$. The domain D(T) is assumed to be a subspace of H. Of course, if $T \in B(H)$, then D(T) = H. Conversely, the closed graph theorem shows that if T is closed and D(T) = H, then $T \in B(H)$, so closed unbounded operators are never defined on all of H. The vast majority of the operators that occur in applications are closed or at least have closed extensions, so the added flexibility of a domain D(T), not necessarily equal to the whole space, is a crucial part of the setup. More generally, the same argument, applied to the Hilbert space $H_0 = D(T)$, shows that a closed unbounded operator can never have a closed domain. Typically, domains of unbounded operators will be dense subspaces. For example, the formal operator Tf = f' on $L^2(\mathbb{R})$ could be given the domain $D(T) = C_0^{\infty}(\mathbb{R})$.

The presence of domains is the main reason why unbounded operators can become quite awkward to deal with. It must always be taken into account when manipulating operators. For example, if S, T are linear operators on H, then we define sum and product as follows:

$$D(S+T) := D(S) \cap D(T) \quad (S+T)x := Sx + Tx, D(ST) := \{x \in D(T) : Tx \in D(S)\} \quad (ST)x := S(Tx)$$

Next, we want to define an adjoint operator T^* . We will assume that T is *densely defined*, that is, $\overline{D(T)} = H$. The following definition looks natural:

$$D(T^*) = \{ x \in H : \text{ There exists } z = z_x \in H \text{ such that} \\ \langle x, Ty \rangle = \langle z, y \rangle \text{ for all } y \in D(T) \}, \\ T^*x := z \qquad (x \in D(T^*))$$

The assumption that T is densely defined makes sure that such a z, if it exists at all, is unique, so this is well defined. Notice that we have defined $D(T^*)$ as the largest set of vectors x for which T can be moved over to the other argument in the scalar product in the expression $\langle x, Ty \rangle$. As before, we call T^* the *adjoint operator* (of T).

Exercise 11.1. Prove that $D(T^*)$ is a subspace and that T^* is a linear operator. Also, prove that if $T \in B(H)$, then this new definition

just recovers the operator $T^* \in B(H)$ that was introduced earlier, in Chapter 6.

One possible concern about this definition is the possibility of $D(T^*)$ being rather small, and, indeed, it can happen that $D(T^*) = 0$, and then we don't really get any operator at all. We'll discuss this in more detail later.

Definition 11.1. The graph of an operator T is the set $G(T) = \{(x, Tx) : x \in D(T)\} \subseteq H \oplus H.$

We have used this notion before, in the closed graph theorem. Notice that G(T) is in fact a subspace of $H \oplus H$. Obviously, the operator, including its domain, can be reconstructed from $G(T) \subseteq H \oplus H$: we have

 $D(T) = \{ x \in H : (x, y) \in G(T) \text{ for some } y \in H \},\$

and then, given $x \in D(T)$, we can recover y = Tx as the unique $y \in H$ with $(x, y) \in G(T)$.

We now introduce a further generalization of the notion of an operator:

Definition 11.2. A relation (on H) is a linear subspace of $H \oplus H$.

More precisely, this generalizes the notion of an operator if we identify operators T with their graphs $G(T) \subseteq H \oplus H$. Relations have their uses in certain situations but are much less common in mainstream functional analysis than operators. We will not do much with them here. They will be quite helpful for us anyway because certain facts about operators actually become clearer in this more general setting.

We want to think about general relations \mathcal{T} in much the same way as operators. So if $(x, y) \in \mathcal{T}$, we view y as an image of x under \mathcal{T} . The indefinite article is appropriate because an $x \in H$ can now have several images. So, for a quick summary, we can say that relations are the same thing as operators, except that they can be multi-valued. With this in mind, we now adapt some old definitions to the new setting and also introduce some new ones.

Definition 11.3. Let $\mathcal{T} \subseteq H \oplus H$ be a relation on H. We define the *domain, range, null space* (or *kernel*), and *multi-valued part* of \mathcal{T} as follows:

$$D(\mathcal{T}) = \{x \in H : (x, y) \in \mathcal{T} \text{ for some } y \in H\},\$$

$$R(\mathcal{T}) = \{y \in H : (x, y) \in \mathcal{T} \text{ for some } x \in H\},\$$

$$N(\mathcal{T}) = \{x \in H : (x, 0) \in \mathcal{T}\},\$$

$$\mathcal{T}(0) = \{y \in H : (0, y) \in \mathcal{T}\}$$

The *inverse* of \mathcal{T} is the relation $\mathcal{T}^{-1} = \{(y, x) : (x, y) \in \mathcal{T}\}$, and the *adjoint* of \mathcal{T} is defined as

$$\mathcal{T}^* = \{ (u, v) : \langle v, x \rangle = \langle u, y \rangle \text{ for all } (x, y) \in \mathcal{T} \}.$$

Finally, the closure $\overline{\mathcal{T}}$ of a relation \mathcal{T} is just that, the closure of the subspace $\mathcal{T} \subseteq H \oplus H$. We call a relation \mathcal{T} closed if $\overline{\mathcal{T}} = \mathcal{T}$.

Exercise 11.2. Show that \mathcal{T}^* indeed is a relation (synonymously: a subspace of $H \oplus H$) and that $D(\mathcal{T})$, $R(\mathcal{T})$, $N(\mathcal{T})$, $\mathcal{T}(0)$ are subspaces of H.

Exercise 11.3. Find the adjoint \mathcal{T}^* of the relation $\mathcal{T} = 0 \oplus H = \{(0, y) : y \in H\}.$

This definition of the relation adjoint reduces to the one we gave earlier if \mathcal{T} is a densely defined operator. As a first advantage of the relations point of view, we now have a unique adjoint for any relation, including non-densely defined operators. (Similarly, any relation has an inverse and a closure.)

Of course, this adjoint \mathcal{T}^* is a relation, not necessarily an operator, so it is now natural to ask under what circumstances \mathcal{T}^* will actually be an operator.

Exercise 11.4. Show that a relation $\mathcal{T} \subseteq H \oplus H$ is an operator (more precisely: $\mathcal{T} = G(T)$ is the graph of an operator T) if and only $\mathcal{T}(0) = 0$.

Theorem 11.4. $\mathcal{T}^*(0) = D(\mathcal{T})^{\perp}$

Proof. We have $z \in D(T)^{\perp}$ if and only if $\langle z, x \rangle = 0$ for all $(x, y) \in \mathcal{T}$. On the other hand, $z \in \mathcal{T}^*(0)$ if and only if $(0, z) \in \mathcal{T}^*$, and by the definition of the adjoint, this leads to the same condition $\langle z, x \rangle = 0$ for all $(x, y) \in \mathcal{T}$.

Corollary 11.5. The adjoint of a relation \mathcal{T} is an operator if and only if \mathcal{T} is densely defined.

This confirms what was our first impression anyway, namely, that we have to insist on dense domains if we want well defined adjoints in an operator setting.

The definition of the property of being closed again reduces to the one we gave earlier if \mathcal{T} is an operator. The notion of a closure is new to us, but of course it almost suggests itself. If we start with an operator T, then we can of course pass to the associated relation $\mathcal{T} = G(T)$ and then take its closure $\overline{\mathcal{T}} = \overline{G(T)}$. This, however, is not guaranteed to be an operator in general (though usually it will be, the counterexamples

are not natural as examples of operators), that is, it can happen that $\overline{\mathcal{T}}(0) \neq 0$ even though $\mathcal{T}(0) = 0$. (In particular, it is not true, in general, that $\overline{\mathcal{T}}(0) = \overline{\mathcal{T}(0)}$.)

So in the operator setting, if multi-valued relations are not admitted, the corresponding definition becomes more awkward.

Definition 11.6. Let T be an operator on H. We call T closable if its relation closure is an operator. In this case, we call the operator associated with $\overline{T} = \overline{G(T)}$ the closure of T and denote it by \overline{T} .

In other words, \overline{T} is defined as the operator with graph $G(\overline{T}) = \overline{G(T)}$.

As always, the sequence characterizations are often easier to work with, so let me state these, too: First of all, for any relation \mathcal{T} , we have $(x, y) \in \overline{\mathcal{T}}$ if and only if there are sequences $(x_n, y_n) \in \mathcal{T}$ such that $x_n \to x, y_n \to y$. In particular, $y \in \overline{\mathcal{T}}(0)$ if and only if there are sequences $x_n \to 0, y_n \to y$ with $(x_n, y_n) \in \mathcal{T}$.

So the operator T is closable if and only if the conditions $x_n \in D(T)$, $x_n \to 0, Tx_n \to y$ for some $y \in H$ imply that y = 0. If T is continuous, then the first two of these three conditions already imply that $Tx_n \to 0$, so a bounded operator is always closable. In general, if T is closable, then

 $D(\overline{T}) = \{x \in H : \text{ There exists a sequence } x_n \in D(T) \text{ such that}$ $x_n \to x, Tx_n \to y \text{ for some } y \in H\}.$

If $x \in D(\overline{T})$ and y is as above, then $\overline{T}x = y$. The condition that T is closable makes sure that this y is uniquely determined by x, so this is well defined.

Exercise 11.5. Show that a bounded operator $T: D(T) \to H$ is closed if and only if D(T) is a closed subspace of H.

Occasionally, the following reformulation is also useful. Call an operator S an extension of T if $G(S) \supseteq G(T)$. Equivalently, this means that $D(S) \supseteq D(T)$ and Sx = Tx for all $x \in D(T)$. In this case, we also write $S \supseteq T$ (this notation goes well with our general convention to identify operators with their graphs in a relations setting).

Exercise 11.6. Prove that T is closable if and only if T has a closed (operator) extension. If T is closable, then \overline{T} is the smallest closed extension of T.

Theorem 11.7. Let \mathcal{T} be a relation. Then: (a) \mathcal{T}^* is closed; (b) $\mathcal{T}^{**} = \overline{\mathcal{T}}$; (c) $\overline{\mathcal{T}}^* = \mathcal{T}^*$.

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Proof. All three parts follow from the fact that we can reinterpret the adjoint as essentially an orthogonal complement. More precisely, let $J \in B(H \oplus H)$ be the unitary map J(x, y) = (-y, x). Then $\mathcal{T}^* = (J\mathcal{T})^{\perp}$. Since an orthogonal complement is always closed, this gives part (a).

Exercise 11.7. Show that for any set $A \subseteq H \oplus H$, we have $J(A^{\perp}) = (JA)^{\perp}$. In fact, you could also establish the general fact that if U is a unitary map on a Hilbert space K, then $UA^{\perp} = (UA)^{\perp}$ for all $A \subseteq K$.

From this Exercise, we obtain

$$\mathcal{T}^{**} = (J\mathcal{T}^*)^{\perp} = (J(J\mathcal{T})^{\perp})^{\perp} = (JJ\mathcal{T}^{\perp})^{\perp} = \mathcal{T}^{\perp\perp} = \overline{\mathcal{T}},$$

and this is part (b).

It then also follows that $\overline{\mathcal{T}}^* = \mathcal{T}^{***} = \overline{\mathcal{T}^*}$, but \mathcal{T}^* is already closed, by part (a), so this equals \mathcal{T}^* , as claimed in part (c).

Here's another useful fact, which generalizes Theorem 6.2.

Theorem 11.8. $N(\mathcal{T}^*) = R(\mathcal{T})^{\perp}$

Proof. We have $z \in N(\mathcal{T}^*)$ if and only if $(z, 0) \in \mathcal{T}^*$ and this happens if and only if $\langle z, y \rangle = 0$ for all $(x, y) \in \mathcal{T}$, but this is the condition for z to lie in $R(\mathcal{T})^{\perp}$.

Exercise 11.8. Let S, T be relations with $S \subseteq T$. Show that then $T^* \subseteq S^*$.

Theorem 11.9. Let T be an operator. Then T is closable if and only if \mathcal{T}^* is densely defined.

Proof. As we discussed earlier, T is closable if and only if $\overline{\mathcal{T}}(0) = 0$. By Theorems 11.7(b) and 11.4, this space equals $\mathcal{T}^{**}(0) = D(\mathcal{T}^*)^{\perp}$. \Box

We can construct non-closable operators most easily in an abstract fashion:

Exercise 11.9. Fix a dense subspace $D_0 \subsetneq H$ and a vector $x \notin D_0$. Let $D(T) = L(x) \dotplus D_0$, T(cx + y) = cx (where $c \in \mathbb{C}$, $y \in D_0$). Show that T is not closable.

Exercise 11.10. Consider again the operator T from the previous Exercise. Observe first of all that T is densely defined, so T^* is an operator by Corollary 11.5. Show that $D(T^*) = \{x\}^{\perp}$, which is not dense (this again implies that T is not closable, by Theorem 11.9). Conclude also $T^*y = 0$ for all $y \in D(T^*)$.

Exercise 11.11. Let \mathcal{T} be a relation. Prove the following: (a) If $N(\mathcal{T})$ is dense, then $\mathcal{T}^* = D(\mathcal{T}^*) \oplus 0$; put differently, v = 0 for all $(u, v) \in \mathcal{T}^*$ (in a concrete setting, you already encountered this situation in Exercise 11.10).

(b) If $R(\mathcal{T})$ is also dense, then $\mathcal{T}^* = 0 \oplus 0 = \{(0,0)\}.$

Exercise 11.12. Here's a more spectacular example of an operator with non-densely defined T^* . Let $H = L^2(-1, 1)$,

$$D(T) = \left\{ f \in C^{\infty}(-1,1) \cap L^{2}(-1,1) : \left| f^{(n)}(0) \right| \le C_{f} 2^{-n} n! \quad (n \ge 0) \right\}$$
$$(Tf)(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^{n};$$

so T sends f to its Taylor series, and the domain only contains functions for which this series converges uniformly and absolutely. Show that T is a densely defined operator with $D(T^*) = 0$.

Suggestion: Show that N(T) and R(T) are dense, and then apply the result of the previous Exercise.

We call a relation \mathcal{T} self-adjoint if $\mathcal{T}^* = \mathcal{T}$ and symmetric if $\mathcal{T} \subseteq \mathcal{T}^*$. Exercise 11.13. Show that self-adjoint relations are closed. Then show that if \mathcal{T} is symmetric, so is $\overline{\mathcal{T}}$.

Symmetric or self-adjoint relations need not be densely defined. Indeed, you showed in Exercise 11.3 that $\mathcal{T} = 0 \oplus H$ is self-adjoint, and here $D(\mathcal{T}) = 0$. However, if we want to deal with operators exclusively, we must insist that T is densely defined, or else T^* would not be an operator (Corollary 11.5). Therefore, the operator version of the definition we just gave goes as follows:

Definition 11.10. We call an operator T symmetric if T is densely defined and $T \subseteq T^*$. If, in addition, $T = T^*$, then we call T self-adjoint.

More explicitly, the symmetry of a densely defined T is equivalent to the condition $\langle x, Ty \rangle = \langle Tx, y \rangle$ for all $x, y \in D(T)$. If, in addition, we also have $D(T) = D(T^*)$, then T is self-adjoint.

Somewhat informally, we can say that symmetry is the familiar property "T can go anywhere in a scalar product", whereas self-adjointness is a more delicate property and involves the domains of T, T^* more explicitly.

Exercise 11.14. Let T be a symmetric operator. Show that T is closable and that \overline{T} is also symmetric.

Example 11.1. Let $H = L^2(0,1)$ and define Tf = if' on $D(T) = C_0^{\infty}(0,1)$, the smooth functions on (0,1) whose support is a compact

subset of (0, 1). Since these are dense in $L^2(0, 1)$, T is densely defined. It is easy to check that T is symmetric: an integration by parts shows that if $f, g \in C_0^{\infty}(0, 1)$, then

$$\langle f, Tg \rangle = \int_0^1 \overline{f(x)} ig'(x) \, dx = -i \int_0^1 \overline{f'(x)} g(x) \, dx = \langle Tf, g \rangle.$$

However, T is not self-adjoint. The above calculation in fact shows that if f is an arbitrary C^1 function, then we still have $\langle f, Tg \rangle = \langle if', g \rangle$, so $D(T^*)$ is strictly larger than $C_0^{\infty} = D(T)$.

Let us try to find T^* explicitly. First of all, if $f \in AC[0, 1]$, then the integration by parts calculation from above still goes through. See Folland, Real Analysis, Theorem 3.36 and Exercise 3.5.35. The space AC[0, 1] of absolutely continuous (on [0, 1]) functions can be defined in various ways; here is one possible version: $f \in AC[0, 1]$ if and only if there exists $h \in L^1(0, 1)$ such that $f(x) = f(0) + \int_0^x h(t) dt$ for all $x \in [0, 1]$. Absolutely continuous functions are differentiable almost everywhere, and if h is as above, then f' = h almost everywhere. Please see Folland, Section 3.5 for (much) more on absolutely continuous functions.

We conclude that $f \in D(T^*)$ if $f \in AC[0,1]$ and $f' \in L^2(0,1)$, and $T^*f = if'$ for these f. Conversely, assume that $f \in D(T^*)$. This means that there exists $h \in L^2(0,1)$ such that

(11.1)
$$i\int_0^1 \overline{f(x)}g'(x)\,dx = \int_0^1 \overline{h(x)}g(x)\,dx$$

for all $g \in C_0^{\infty}(0, 1)$. Now one possible interpretation of (11.1) is: the distributional derivative of f equals -ih. In particular, $f' \in \mathcal{D}'(0, 1)$ is an integrable function (since $L^2(0, 1) \subseteq L^1(0, 1)$). This implies that $f \in AC[0, 1]$ and h = if', so

(11.2)
$$D(T^*) = \{ f \in AC[0,1] : f' \in L^2(0,1) \}, \quad T^*f = if'.$$

If you are not familiar with the distributional characterization of absolute continuity, then the use of distributions can be avoided. Here's an alternative argument. Suppose that f and h are as in (11.1), and let

(11.3)
$$F(x) = f(x) + i \int_0^x h(t) dt.$$

Clearly, $F \in L^2(0, 1)$. A calculation using the Fubini-Tonelli Theorem and (11.1) shows that $\langle F, g' \rangle = 0$ for all $g \in C_0^{\infty}(0, 1)$. Fix $g_0 \in C_0^{\infty}(0, 1)$ with $\int g_0 = 1$. Also, observe that $h \in C_0^{\infty}(0, 1)$ is of the form h = g'for some $g \in C_0^{\infty}(0, 1)$ if (and only if, but this is not needed here) $\int h = 0$, so we can now rephrase and say that $\langle F, g - cg_0 \rangle = 0$ for all $g \in C_0^{\infty}(0, 1)$, where $c = \int g = \langle 1, g \rangle$. Or, put differently, $\langle F - c_0, g \rangle = 0$

for all $g \in C_0^{\infty}(0, 1)$, and here $c_0 = \langle g_0, F \rangle \in \mathbb{C}$ is a constant (function). However, $C_0^{\infty}(0, 1)^{\perp} = 0$, because C_0^{∞} is dense, so $F = c_0$. Now (11.3) again confirms that (11.2) holds.

In particular, T^* is densely defined, so T is closable. What is its closure?

Exercise 11.15. Use similar arguments to show that

$$D(T^{**}) = \{ f \in AC[0,1] : f' \in L^2(0,1), f(0) = f(1) = 0 \},\$$

$$T^{**}f = if'.$$

Recall also that AC[0, 1] functions are continuous on [0, 1], so it makes sense to evaluate these at 0 and 1.

Let $S = \overline{T} = T^{**}$. Then S is closed and symmetric because $S^* = T^*$ and thus $S^* \supseteq S$ by (11.2). However, S is not self-adjoint, as $D(S^*)$ is strictly larger than D(S). When we make the domain larger (but in such a way that we still have a restriction of S^*), the domain of the adjoint operator will decrease, so perhaps self-adjoint operators can be obtained in this way. It is clear that $D(S^*)$ is too large; in fact, S^* is not even symmetric because $S^{**} = S \not\supseteq S^*$. However, the intermediate domains

$$D(S_a) = \{ f \in AC[0,1] : f(1) = e^{ia} f(0) \}, \qquad S_a f = if'$$

work: S_a is self-adjoint for every $a \in [0, 2\pi)$ (we don't want to prove this here, but you can try to give a proof that is modeled on the discussion above). Notice that $S \subseteq S_a \subseteq S^*$ for all a.

This situation is typical. It is often easy to find domains on which operators are symmetric, but to build self-adjoint operators, the domains must be chosen very carefully. The *von Neumann theory* provides a systematic approach to these issues; we will not discuss it here. Instead, we will prove the following abstract criterion.

Theorem 11.11. Let T be a symmetric operator, and let $z \in \mathbb{C} \setminus \mathbb{R}$. Then the following statements are equivalent: (a) T is self-adjoint;

(b) T is closed and $N(T^* - z) = N(T^* - \overline{z}) = 0;$ (c) $R(T - z) = R(T - \overline{z}) = H.$

Here, as usual, T - z really means T - zI, with Ix = x being the identity operator (and the multiplicative identity e = I of the C^* -algebra B(H)). For such sums (or differences) of an operator with a *bounded* operator, the domains don't make much trouble: we have $D(T - z) = D(T) \cap D(zI) = D(T) \cap H = D(T)$.

We will also make use of the following fact: If T is a densely defined operator and $z \in \mathbb{C}$, then $(T - z)^* = T^* - \overline{z}$.

Exercise 11.16. Prove this.

Proof. (a) \implies (b): T is closed because $T = T^*$ and adjoints are always closed (Theorem 11.7). Suppose that $x \in N(T^* - z) = N(T - z)$. Then

$$\overline{z}\langle x,x\rangle = \langle Tx,x\rangle = \langle x,Tx\rangle = z\langle x,x\rangle,$$

so x = 0. Of course, a similar argument works for $N(T^* + z)$, so we have established (b).

(b) \implies (c): By Theorem 11.8, $R(T-z)^{\perp} = N(T^* - \overline{z}) = 0$, so R(T-z) is dense. So it now suffices to show that this space is closed. Let $y_n \in R(T-z)$, so $y_n = (T-z)x_n$ with $x_n \in D(T)$, and suppose that $y_n \to y$. Write z = a + ib; by assumption, $b \neq 0$. If $u \in D(T)$, then

$$\|(T-z)u\|^{2} = \langle (T-a-ib)u, (T-a-ib)u \rangle$$
$$= \|(T-a)u\|^{2} + b^{2}\|u\|^{2}$$

because $T^* \supseteq T$, so $\langle u, (T-a)u \rangle = \langle (T-a)u, u \rangle$. It follows that

$$||u|| \le \frac{1}{|b|} ||(T-z)u||,$$

and by applying this to $u = x_m - x_n$, we see that x_n is a Cauchy sequence, so $x = \lim x_n$ exists. Since Tx_n also converges, to y + zx, and T is closed, we conclude that $x \in D(T)$ and Tx = y + zx or $y = (T - z)x \in R(T - z)$, as desired. An analogous argument handles $R(T - \overline{z})$.

(c) \Longrightarrow (a): Let $x \in D(T^*)$. By hypothesis, we can find a $y \in D(T)$ with $(T-z)y = (T^*-z)x$. Since $T \subseteq T^*$, we have $x - y \in N(T^*-z)$. However, $N(T^*-z) = R(T-\overline{z})^{\perp} = 0$ (by Theorem 11.8 and assumption), so $x = y \in D(T)$. We have shown that $D(T^*) \subseteq D(T)$, so $D(T^*) = D(T)$ since T is symmetric.

Definition 11.12. Let T be a closed operator. Define

$$\rho(T) = \{ z \in \mathbb{C} : N(T - z) = 0, R(T - z) = H \}$$

$$\sigma(T) = \mathbb{C} \setminus \rho(T).$$

We call $\rho(T)$ the resolvent set and $\sigma(T)$ the spectrum of T.

Notice that if $z \in \rho(T)$, then $(T-z)^{-1} \in B(H)$. This follows from the closed graph theorem because $(T-z)^{-1}$ is a closed operator that is defined everywhere. Here we use the fact that an injective operator S is closed if and only if S^{-1} is closed; in fact, this is obvious because $G(S) = \{(x, Sx) : x \in D(S)\}$ and $G(S^{-1}) = \{(Sx, x) : x \in D(S)\}$.

Conversely, if T - z is invertible as a map and $(T - z)^{-1} \in B(H)$, then obviously $z \in \rho(T)$.

These remarks confirm that the definition is natural. The resolvent set consists of those $z \in \mathbb{C}$ for which T - z is invertible as a map and the inverse map lies in B(H), and this is a direct generalization of our earlier definition for bounded operators. As before, we call R(z) = $(T - z)^{-1}$ ($z \in \rho(T)$) the resolvent of T.

Proposition 11.13. $\rho(T)$ is an open subset of \mathbb{C} .

This is proved as in the case of bounded operators. If $T - z_0$ is invertible in B(H), then we can write $T - z = (T - z_0)(1 + (z - z_0)(T - z_0)^{-1})$ (as usual, the domains require constant attention, but they do not cause any trouble in this formula) and then use the Neumann series to show that the second factor is invertible in B(H) if $|z - z_0|$ is small. See our discussion in Chapter 7, especially Corollary 7.5 and Theorem 7.7(a).

Proposition 11.14 (First resolvent identity). Let T be a closed operator and $w, z \in \rho(T)$. Then

$$R(w) - R(z) = (w - z)R(w)R(z);$$

in particular, R(w) and R(z) commute.

Proof. We have

$$(w-z)R(w)R(z) = R(w)(T-z - (T-w))R(z) = R(w) - R(z),$$

which appears to verify the claim. However, this is a formal calculation and we also need to take the domains into account. More precisely, the domain of R(w)((T-z) - (T-w))R(z) is the space of those $x \in H$ for which $R(z)x \in D(T)$, but, fortunately, this is all of H because R(z), being the inverse of T-z, has range D(T-z) = D(T). So the above calculation is sound.

Exercise 11.17. Here's an illustration of the kind of trouble we might run into if we let our guard down and just manipulate formally, without watching domains: Show that $RS + RT \subseteq R(S + T)$, and give an example (perhaps an easy abstract example) where the two sides don't have the same domain.

Corollary 11.15. Let T be self-adjoint. Then $\sigma(T) \subseteq \mathbb{R}$.

Proof. By combining (b) and (c) of Theorem 11.11, we see that N(T - z) = 0, R(T - z) = H for every $z \notin \mathbb{R}$.

The following example once again demonstrates the dramatic effect that domain issues can have.

Example 11.2. Consider again the operator $f \mapsto if'$ on $L^2(0,1)$, on the following domains:

$$D(S) = \{ f \in AC[0,1] : f' \in L^2(0,1) \},\$$

$$D(T) = \{ f \in D(S) : f(0) = 0 \}$$

So S is the operator T^* from Example 11.1.

Exercise 11.18. Prove that both operators are closed.

I claim that

$$\sigma(S) = \mathbb{C}, \qquad \sigma(T) = \emptyset.$$

The claim on $\sigma(S)$ is very easy to confirm. Just notice that $e_z(x) = e^{-izx} \in D(S)$ for all $z \in \mathbb{C}$ and $(S-z)e_z = 0$.

To find $\sigma(T)$, fix $z \in \mathbb{C}$ and let

$$(R_z f)(x) = -ie^{-izx} \int_0^x e^{izt} f(t) dt.$$

This is defined for all $f \in L^2(0, 1)$, and in fact $(R_z f)(x)$ is an absolutely continuous function of $x \in [0, 1]$. In particular, $R_z f \in L^2(0, 1)$. An easy calculation shows that

$$(R_z f)'(x) = -iz(R_z f)(x) - if(x)$$

(almost everywhere). This implies that $(R_z f)' \in L^2(0,1)$, and since clearly $(R_z f)(0) = 0$, it follows that $R_z f \in D(T)$. Moreover, $(T - z)R_z = 1$ (note that the observations about R_z mapping to D(T) are needed here to be able to define the left-hand side on all of H), so R(T - z) = H. Similar arguments (use an integration by parts!) show that $R_z(T - z)f = f$ for all $f \in D(T)$, so we also obtain N(T - z) = 0(since $R_z 0 = 0$). Putting things together, we see that $z \in \rho(T)$, and $z \in \mathbb{C}$ was arbitrary here.

We want to formulate and prove the Spectral Theorem for *unbounded* self-adjoint operators also. From a purely formal point of view, things look very familiar:

Theorem 11.16 (The Spectral Theorem for self-adjoint operators). Let T be a self-adjoint operator. Then there exists a unique spectral resolution E (on the Borel sets of $\sigma(T)$) such that

(11.4)
$$T = \int_{\sigma(T)} t \, dE(t).$$

However, we must tread very carefully here. If T is unbounded, then $\sigma(T)$ could be an unbounded subset of \mathbb{R} (in fact, as we will prove later, $\sigma(T)$ is never bounded unless $T \in B(H)$), and thus (11.4) involves a

new kind of integral that we haven't even defined yet (the integrand is an unbounded function).

Clearly, we first need to address this issue, and we will do this in an abstract setting. So let $E : \Omega \to B(H)$ be a resolution of the identity on an arbitrary space (Ω, \mathcal{M}) . We want to extend our earlier definition of $\int_{\Omega} f \, dE$ to unbounded measurable functions f. If $f : \Omega \to \mathbb{C}$ is such an arbitrary measurable function, we let

$$D_f = \left\{ x \in H : \int_{\Omega} |f(t)|^2 \, d \|E(t)x\|^2 < \infty \right\}.$$

As a preliminary, we observe the following:

Lemma 11.17. D_f is a dense subspace of H. If $x \in D_f$ and $y \in H$, then

(11.5)
$$\int_{\Omega} |f| \, d|\mu_{y,x}| \le ||y|| \left(\int_{\Omega} |f|^2 \, d\mu_{x,x}\right)^{1/2}$$

Here, we use the same notation as in Chapter 10: $\mu_{y,x}$ denotes the complex measure $\mu_{y,x}(\omega) = \langle y, E(\omega)x \rangle$. We sometimes write $d\mu_{y,x} = d\langle y, Ex \rangle$ instead.

Proof. Suppose that z = x + y, with $x, y \in D_f$. Then, for all $\omega \in \mathcal{M}$, we have

$$||E(\omega)z||^{2} \leq (||E(\omega)x|| + ||E(\omega)y||)^{2} \leq 2||E(\omega)x||^{2} + 2||E(\omega)y||^{2}.$$

This says that $\mu_{z,z}(\omega) \leq 2\mu_{x,x}(\omega) + 2\mu_{y,y}(\omega)$, so $z \in D_f$. If $c \in \mathbb{C}$ and $x \in D_f$, then $\mu_{cx,cx}(\omega) = |c|^2 \mu_{x,x}(\omega)$, so $cx \in D_f$ also.

To prove that D_f is dense, put $\omega_n = \{t \in \Omega : |f(t)| < n\}$. If $y \in R(E(\omega_n))$, then $\mu_{y,y}(\omega_n^c) = 0$ (why?), so

$$\int_{\Omega} |f|^2 d\mu_{y,y} = \int_{\omega_n} |f|^2 d\mu_{y,y} \le n^2 ||y||^2 < \infty,$$

and thus $y \in D_f$. I now claim that $E(\omega_n)x \to x$ for arbitrary $x \in H$. To verify this, notice that $||x - E(\omega_n)x||^2 = \mu_{x,x}(\omega_n^c)$. This goes to zero because the sets ω_n^c decrease to the empty set: $\omega_1^c \supseteq \omega_2^c \supseteq \ldots$, $\bigcap \omega_n^c = \emptyset$ (you can also apply Monotone Convergence to the functions $1 - \chi_{\omega_n^c} = \chi_{\omega_n}$).

We first prove (11.5) for bounded f. Write $d|\mu_{y,x}| = u d\mu_{y,x}$, with |u| = 1. Then

$$\begin{split} \int_{\Omega} |f| \, d|\mu_{y,x}| &= \int_{\Omega} u|f| \, d\mu_{y,x} = \langle y, \Psi(u|f|)x \rangle \\ &\leq \|y\| \, \|\Psi(u|f|)x\| = \|y\| \left(\int_{\Omega} |f|^2 \, d\mu_{x,x}\right)^{1/2}, \end{split}$$

as claimed. Here, we make use of the notation $\Psi(g) = \int g \, dE$ (as in Chapter 10).

For general measurable f, we can apply this to $f_n = \chi_{\{|f| < n\}} f$ and use Monotone Convergence to pass to the limit on both sides of (11.5). \Box

Theorem 11.18. (a) There exists a unique linear operator $T_f : H \to H$ with $D(T_f) = D_f$ and

(11.6)
$$\langle y, T_f x \rangle = \int_{\Omega} f(t) \, d\mu_{y,x}(t)$$

for all $x \in D_f$, $y \in H$. (b) If $x \in D_f$, then

$$||T_f x||^2 = \int_{\Omega} |f(t)|^2 d\mu_{x,x}(t).$$

(c)
$$T_f T_g \subseteq T_{fg}$$
 and $D(T_f T_g) = D_g \cap D_{fg}$;
(d) $T_f^* = T_{\overline{f}}$; in particular, T_f is closed.

This allows us to define $\int_{\Omega} f \, dE := T_f$. Since we are again using (11.6) as the defining property of this operator, it is clear that this reproduces our earlier definition from Chapter 10 if $f \in L^{\infty}(\Omega, E)$. Here, we also use the observation that $D_f = H$ if f is (essentially) bounded. Theorem 11.19 below will discuss these issues again.

The map $f \mapsto T_f$ has similar properties as before, but, as usual, the domains now need to be watched constantly. Part (c) is the new version of multiplicativity, and it can also be proved that $T_f + T_g \subseteq T_{f+g}$ and $cT_f = T_{cf}$ (if $c \neq 0$).

Note also that (11.5) from Lemma 11.17 makes sure that the righthand side of (11.6) is well defined for $x \in D_f$.

Proof. (a) Uniqueness is clear because (11.6) determines $T_f x$. To prove existence, we fix $x \in D_f$ and consider the map $y \mapsto \overline{\int f d\mu_{y,x}}$. This map is a linear functional, and by (11.5), it is also bounded, of norm at most $\left(\int |f|^2 d\mu_{x,x}\right)^{1/2}$. Hence the Riesz Representation Theorem provides a vector $z = z_x \in H$, of at most this norm, such that $\int f d\mu_{y,x} = \langle y, z \rangle$. Let $T_f x = z$. Since $\mu_{y,x}$ depends linearly on x, this defines a *linear* map $T_f : D_f \to H$.

(b) As just observed,

(11.7)
$$||T_f x||^2 \le \int_{\Omega} |f|^2 d\mu_{x,x} \quad (x \in D_f).$$

Let f_n again denote the truncated function

$$f_n(t) = \begin{cases} f(t) & |f(t)| < n \\ 0 & |f(t)| \ge n \end{cases}$$

Then $D_{f-f_n} = D_f$, and now (11.7) together with Dominated Convergence shows that $||T_f x - T_{f_n} x|| = ||T_{f-f_n} x|| \to 0$. Since f_n is bounded, the asserted identity holds for f_n , and now another passage to the limit yields the claim for f as well.

(c) We first deal with the case when f is bounded. Then $D_g \subseteq D_{fg}$. If $x \in D_g$ and $y \in H$, then

$$\langle y, T_f T_g x \rangle = \langle T_{\overline{f}} y, T_g x \rangle = \int_{\Omega} g \, d \langle T_{\overline{f}} y, Ex \rangle,$$

$$\langle y, T_{fg} x \rangle = \int_{\Omega} fg \, d \langle y, Ex \rangle.$$

If g is also bounded, then we know that $T_f T_g = T_{fg}$ (Theorem 10.3), so the two integrals are also equal to each other in this case. Now the Dominated Convergence Theorem lets us extend this equality to general measurable functions g (by applying the usual technique of truncating g and passing to the limit), so

(11.8)
$$T_f T_g x = T_{fg} x \qquad (x \in D_g).$$

Since $D(T_fT_g) = D_g$ if f is bounded, this is what we claimed in the Theorem, for bounded f.

To remove this restriction, first of all notice that if f is bounded and $x \in D_g$, then

(11.9)
$$\int_{\Omega} |f|^2 d\langle T_g x, ET_g x \rangle = \int_{\Omega} |fg|^2 d\langle x, Ex \rangle.$$

The usual truncation plus limit trick shows that this identity in fact holds for all measurable f. By definition, $D(T_fT_g)$ consists of those $x \in D_g$ for which $T_g x \in D_f$. By (11.9), this set coincides with $D_g \cap D_{fg}$, as claimed.

If x is from this set, define, as usual, bounded truncations f_n . Then, by the argument discussed in the proof of part (b), $T_{f_n}T_gx \to T_fT_gx$, $T_{f_ng}x \to T_{fg}x$, so we can use (11.8) with f_n in place of f (recall that (11.8) was only derived for bounded f!) and pass to the limit to obtain the full claim.

(d) If $x \in D_f$ and $y \in D_{\overline{f}} = D_f$, then

$$\langle y, T_f x \rangle = \int_{\Omega} f \, d\mu_{y,x} = \overline{\int_{\Omega} \overline{f} \, d\mu_{x,y}} = \overline{\langle x, T_{\overline{f}} y \rangle} = \langle T_{\overline{f}} y, x \rangle.$$

This says that $y \in D(T_f^*)$ and $T_f^* \supseteq T_{\overline{f}}$.

Conversely, suppose that $y \in D(\mathring{T}_{f}^{*})$. Let again $\omega_{n} = \{t \in \Omega : |f(t)| < n\}$ and $f_{n} = \chi_{\omega_{n}} f$. I claim that

(11.10)
$$T_{\overline{f}_n}y = E(\omega_n)T_f^*y.$$

Indeed, f_n is bounded, so, for arbitrary $x \in H$, we have

$$\langle T_{\overline{f}_n} y, x \rangle = \langle y, T_{f_n} x \rangle = \int_{\Omega} f_n \, d\mu_{y,x} = \int_{\omega_n} f \, d\mu_{y,x},$$
$$\langle E(\omega_n) T_f^* y, x \rangle = \langle y, T_f E(\omega_n) x \rangle = \int_{\Omega} f \, d\mu_{y,E(\omega_n)x}.$$

Now $\mu_{y,E(\omega_n)x}(\omega) = \mu_{y,x}(\omega \cap \omega_n)$, so the two integrals are equal to each other. This property of μ also shows that $E(\omega_n)x \in D_f$, so there are no problems with the domains in the second line of the displayed equations.

Now (11.10) implies that

$$\int_{\Omega} |f_n|^2 \, d\mu_{y,y} = \|E(\omega_n)T_f^*y\|^2 \le \|T_f^*y\|^2,$$

and the Monotone Convergence Theorem lets us conclude that $y \in D_{\overline{f}}$, as desired.

Finally, $T_f = T_{\overline{f}}^*$ is closed by Theorem 11.7.

Theorem 11.19. Let $f : \Omega \to \mathbb{C}$ be a measurable function. Then $D(T_f) = H$ if and only if f is essentially bounded.

Proof. Obviously, $D_f = H$ if f is (essentially) bounded. Conversely, if $D_f = H$, then $T_f \in B(H)$ by the Closed Graph Theorem. Let $\omega_n = \{t \in \Omega : |f(t)| \ge n\}$. Theorem 11.18(b) shows that $||T_f x|| \ge n ||x||$ for all $x \in R(E(\omega_n))$, so we must have $E(\omega_n) = 0$ for all large n. \Box

We have clarified the precise meaning of this new version of the Spectral Theorem (for unbounded self-adjoint operators), and we are also in a position to prove it now.

Proof of Theorem 11.16. The idea is quite simple, but the technical details are perhaps slightly unpleasant and so I will be a bit light on the details here. If T is self-adjoint, then $i \notin \sigma(T)$, by Corollary 11.15, so $R = (T - i)^{-1} \in B(H)$.

Exercise 11.19. Prove that $R^* = (T+i)^{-1}$.

Moreover, by Exercise 11.19 and Proposition 11.14, $RR^* = R^*R$, so R is a bounded normal operator.

By the Spectral Theorem for these (Theorem 10.5),

$$(T-i)^{-1} = \int_{\sigma(R)} z \, dF(z)$$

for some spectral resolution F. We want to "change variables" from z to t, where 1/(t-i) = z. So let $\varphi(t) = 1/(t-i)$ and put $E(M) = F(\varphi(M \setminus \{i\}))$. (We remove the point i here to have a meaningful definition, but there really is no issue at all; see the comment in part (b) of the following Exercise.)

Exercise 11.20. (a) Show that this defines a new resolution of the identity E.

(b) Show that $\int z \, dF(z) = \int \frac{1}{t-i} dE(t)$. Remark: Notice that F, being the spectral resolution of a bounded operator, is supported by a *compact* set, so there is a disk D about i with E(D) = 0, and thus the integrand 1/(t-i) is an essentially bounded function and $\int dE/(t-i) \in B(H)$, as required.

We of course expect that $T - i = R^{-1} = \int (t - i) dE$, so $T = \int t dE$, but, as always, it is good practice to be suspicious about these formal manipulations, and we will again need to address domain issues here. Moving on to the rigorous discussion, we let $S = \int t dE(t)$ and notice that Theorem 11.18(c) implies that (S - i)R = 1. Since R maps onto D(T), this identity in particular shows that $D(S) \supseteq D(T)$. Moreover, if $x \in D(T)$ and thus x = Ry for some $y \in H$, then Sx = SRy =y + iRy = TRy = Tx. Hence $S \supseteq T$, and by taking adjoints, we see that in fact $S^* \subseteq T \subseteq S$; in particular, $S^* = \int \overline{t} dE(t)$ is a symmetric operator (recall that S is closed, so $S^{**} = S$).

Exercise 11.21. Let E be a resolution of the identity on Ω , and let $f: \Omega \to \mathbb{C}$ be a measurable function. Assume that $A = \int_{\Omega} f \, dE$ is a symmetric operator. Show that then A is self-adjoint. *Hint:* Show that $E(\{t \in \Omega : f(t) \notin \mathbb{R}\}) = 0$ if A is symmetric.

So it now follows that S = T, and this gives a representation of the type $T = \int_{\mathbb{C}} t \, dE(t)$. We must also show that E is supported by $\sigma(T)$. We leave this final touch to the reader; the argument is quite similar to analogous discussions from Chapter 10.

Exercise 11.22. Provide details, along the following lines: First of all, argue that it suffices to show that if $E(B_r(z)) \neq 0$ for all r > 0, then $z \in \sigma(T)$. Then establish this property, by constructing a sequence $x_n \in D(T)$ with $||x_n|| = 1$ and $(T - z)x_n \to 0$.

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Finally, we sketch a possible proof of the uniqueness assertion: We can, conversely, go from a representation $T = \int t \, dE(t)$ of T to a representation $(T - i)^{-1} = \int z \, dF(z)$ of the resolvent, by a change of variables again. Moreover, it is possible to recover E from F. Since we know that F is unique (Theorem 10.5), E must be unique, too.

From the Spectral Theorem, we again obtain a functional calculus for self-adjoint operators. More precisely, if $T = \int t \, dE(t)$ and $f: \sigma(T) \to \mathbb{C}$ is measurable, then we put $f(T) = \int f(t) \, dE(t)$. Note that this is well defined even if both f and T are unbounded. If f is (essentially) bounded, then $f(T) \in B(H)$, whether or not T is bounded. In fact, it was exactly this property of self-adjoint operators (with f(t) = 1/(t-i)) that made our proof of the Spectral Theorem work.

Unbounded self-adjoint operators also have spectral representations, that is, they are unitarily equivalent to multiplication by the variable on a sum of $L^2(\mathbb{R}, d\rho)$ spaces, but we will not develop this result here.

Exercise 11.23. Let ρ be a finite (positive) Borel measure on \mathbb{R} . Let

$$D(M) = \{ f \in L^2(\mathbb{R}, d\rho) : tf(t) \in L^2(\mathbb{R}, d\rho) \},\$$

$$(Mf)(t) = tf(t).$$

Prove that M is a self-adjoint operator on $L^2(\mathbb{R}, d\rho)$.

Theorem 11.20. Let T be a self-adjoint operator. Then $T \in B(H)$ if and only if $\sigma(T)$ is a bounded set.

Exercise 11.24. Prove this. One direction is of course already known to us, and the other direction follows quickly from the Spectral Theorem and Theorem 11.18(b).

One may also wonder if self-adjoint *relations* (rather than operators) have a similar spectral theory. This is clarified by the following result.

Theorem 11.21. Let \mathcal{T} be a self-adjoint relation on H. Then $H = H_1 \oplus H_2$, with $H_1 = \overline{D(\mathcal{T})}$, $H_2 = \mathcal{T}(0)$, and, correspondingly, $\mathcal{T} = \mathcal{T}_1 \oplus \mathcal{T}_2$, with $\mathcal{T}_j = \mathcal{T} \cap (H_j \oplus H_j)$. More precisely, $\mathcal{T}_1(0) = 0$, so \mathcal{T}_1 is a self-adjoint operator on H_1 , and $\mathcal{T}_2 = 0 \oplus H_2$.

Exercise 11.25. Let \mathcal{T}_j , j = 1, 2, be a relation on H_j . Suppose that $H = H_1 \oplus H_2$ and $\mathcal{T} = \mathcal{T}_1 \oplus \mathcal{T}_2$. Show that then $\mathcal{T}^* = \mathcal{T}_1^* \oplus \mathcal{T}_2^*$. In particular, \mathcal{T} is self-adjoint if and only if \mathcal{T}_1 and \mathcal{T}_2 are.

So a self-adjoint relation is always a self-adjoint operator on the smaller Hilbert space $H_1 = \overline{D(\mathcal{T})}$, and it is purely multi-valued on the orthogonal complement H_2 . Or, put differently, if we divide out the multi-valued part H_2 , then we obtain a self-adjoint operator.

Proof. Theorem 11.4 shows that $\mathcal{T}(0) = D(\mathcal{T})^{\perp}$, so H_1 , H_2 are indeed orthogonal complements of one another. Moreover, it is clear that $\mathcal{T}_1 \oplus$ $\mathcal{T}_2 \subseteq \mathcal{T}$. Conversely, if $(x, y) \in \mathcal{T}$, then, with $z = P_{H_2}y$, we have $y - z = (1 - P_{H_2})y = P_{H_1}y \in H_1$, and since $z \in \mathcal{T}(0)$, it is also true that $(x, y - z) \in \mathcal{T}$ and in fact $(x, y - z) \in \mathcal{T}_1$ since also $x \in D(\mathcal{T}) \subseteq H_1$. Thus (x, y) = (x, y - z) + (0, z) is a decomposition of the required type. The remaining statements follow from the fact that $H_2 = \mathcal{T}(0)$. \Box

Exercise 11.26. Let T be a linear operator. Let, for $x, y \in D(T)$,

$$[x, y] = \langle x, y \rangle + \langle Tx, Ty \rangle.$$

Prove that this defines a new scalar product on D(T). Then show that T is closed if and only if D(T) is complete with respect to $[\cdot, \cdot]$.

Exercise 11.27. Prove that the operator T from Example 11.1 is not bounded. Do this directly, by constructing functions $f_n \in C_0^{\infty}(0,1)$ with $||f_n|| = 1$, $||f'_n|| \to \infty$.

Exercise 11.28. Let T be a self-adjoint operator and let $M \subseteq H$ be a closed subspace. We call M a *reducing subspace* if $D(T) = (M \cap D(T)) + (M^{\perp} \cap D(T))$ and both M and M^{\perp} are invariant under T: if $x \in M \cap D(T)$, then $Tx \in M$, and similarly on $M^{\perp} \cap D(T)$. Roughly speaking, these conditions say that T can be split into two parts, one on M and a second part on M^{\perp} .

(a) Show that M is reducing if and only if $PT \subseteq TP$, where P denotes the projection onto M.

(b) Let E be the spectral resolution of T. Show that R(E(B)) is a reducing subspace for every Borel set $B \subseteq \mathbb{R}$. *Hint:* Theorem 11.18(c)

Exercise 11.29. Show that if T is self-adjoint, $z \notin \sigma(T)$, and f(t) = 1/(t-z), then f(T) = R(z) (as expected).

Exercise 11.30. Similarly, show that if $f(t) = t^2$, then f(T) agrees with the direct definition of $T^2 = TT$ that was discussed at the beginning of this chapter. (More generally, if f = p is a polynomial, then the functional calculus just reproduces the direct definition of p(T).)