Unbounded Operator Notes

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1. Unbounded Operators

Until now, our concentration has been on bounded (i.e. continuous) operators. But many important operators, differential operators among them, are unbounded, defined on a dense subset of a Hilbert space but not on the whole space.

We discussed a few properties of such operators—closed operators— in Section **??** and we continue that discussion here.

A primary user-group of this material, physicists thinking about quantum mechanics, employs a slightly different notation from that used by most mathematicians, and that can lead to communication problems. For instance an inner product $\langle\, x\,,\, y \,\rangle$ is denoted $\langle\, y \,|\, x \,\rangle$, so to these physicists an inner product is conjugate linear in the first "slot" and linear in the second. Also, it is pretty universal for physicists to employ λ^* rather than $\overline{\lambda}$ to denote complex conjugation of the number λ.

Using this vocabulary a vector w is indicated by what is termed a **ket**, $|\,\mathbf{w}\,\rangle = w$, while a functional corresponding to inner product against vector v is called a **bra**, $\langle\,\mathbf{v}\,| = \langle\,\cdot\,,\, v\,\rangle$. Thus we have a **bracket**, a number, given by

$$\langle\, v\,|\;|\, w\,\rangle = \langle\, v \,|\, w\,\rangle = \langle\, w\,,\, v\,\rangle.$$

The map that identifies $\mathcal{H}$ with its dual $\mathcal{H}'$ is conjugate linear. Thus

$$\langle\, f + \lambda\, g \,| = \langle\, f\,| + \lambda^* \langle\, g\,|.$$

Bras and kets are frequently transformed into each other, and it is this conjugate linear identification that does the job.

If Ψ is an operator, the symbol $\langle\, v\,|\,\Psi$ denotes the functional defined by

$$\langle\, v \,|\, \Psi\,(\,|\, w\,\rangle\,) = \langle\, \Psi(w)\,,\, v\rangle$$

and this number is usually denoted $\langle\, v\,|\,\Psi\,|\, w\,\rangle$. The notation is linear in the "spots" occupied by Ψ and w (individually) and conjugate linear in the location of v.

$|\, v\,\rangle\,\langle\, w\,|$ is intended to represent a linear operator mapping onto the span of v related to a projection. Specifically,

$$|\, v\,\rangle\,\langle\, w\,|\,(\,|\, u\,\rangle\,) = \langle\, w\,|\, u\,\rangle\,|\, v\,\rangle = \langle\, u\,,\, w\,\rangle\, v$$

and if $w = v$ and a unit vector this is the projection onto the span of v.

If you see symbols rather than vectors inside a bra or a ket, the intent is to label instances of a vector or functional. A mathematician might use subscripts or superscripts on a generic vector symbol for this. For instance, if you see an indexed ket $|\, i, j\,\rangle$ the intent is that there are vectors $v_{i,j}$ for which $|\, i, j\,\rangle = |\, v_{i,j}\,\rangle = v_{i,j}$. Or if λ is an eigenvalue of an operator the ket $|\,\lambda\rangle$ would denote an eigenvector for λ.

Apparently context and habit helps the expert user keep this kind of shorthand straight, but it is a *common* source of confusion for the beginner.

A function T is often defined as a set of ordered pairs where each first component is associated with exactly one ordered pair in this set. The set of first components is the domain of the function, and the set consists of ordered pairs of the form $(x, T(x))$. In other words, with this definition a function actually *is* its graph $\gamma(T)$. The distinction is that $\gamma(T)$ has subspace topology from a product space, while T

itself has no topology or other structures associated with it. It is rarely relevant to draw this distinction.

For each such T we will let $\mathcal{D}_T$ denote the domain of T and indicate the image $T(\mathcal{D}_T)$ of T by $\mathcal{R}_T$. Unless otherwise noted, whenever we use this notation for domain and range we presume T to be linear on vector space $\mathcal{D}_T$.

Two functions are equal if *the two domains and all function values coincide.*

For two functions S and T we have a partial ordering given by containment. So $S \subset T$ provided that T is an extension of S to larger domain. In particular, $\mathcal{D}_S \subset \mathcal{D}_T$ and $S(x) = T(x)$ for every $x \in \mathcal{D}_S$.

Generally, we define $S + T$ in the obvious way, with domain $\mathcal{D}_{S+T} = \mathcal{D}_S \cap \mathcal{D}_T$. And $S \circ T$ is defined with domain $\mathcal{D}_{S \circ T} = \{\, x \in \mathcal{D}_T \mid T(x) \in \mathcal{D}_S \,\}$.

When T is one-to-one we define T^{-1} for the members $\mathcal{D}_{T^{-1}} = \mathcal{R}_T$ of $\mathcal{H}$ by $T^{-1}(T(x)) = x$. Recall from Exercise **??** that if T is closed, so is T^{-1}.

Because of domain confusion we use the word "commute" cautiously when applied to unbounded operators.

Note that $T \circ S$ has domain consisting of those $x \in \mathcal{D}_S$ for which $S(x) \in \mathcal{D}_T$, while $S \circ T$ has domain consisting of those $x \in \mathcal{D}_T$ for which $T(x) \in \mathcal{D}_S$. These domains will often be different, and even when they are equal their common domain could easily contain just the zero vector. It is unclear how useful a relation such as $S \circ T = T \circ S$ might be. If T is one-to-one, and so possesses an inverse function $T^{-1} \colon \mathcal{R}_T \to \mathcal{D}_T$ the compositions $T \circ T^{-1}$ and $T^{-1} \circ T$ are both the identity, but possibly on different subsets of $\mathcal{H}$. These maps cannot be said to commute in general.

With these issues in mind, we define a relation between two operators B and T that recovers part of what we use "commutativity" for, but with restrictions, and which is *not* symmetric.

We say **B commutes with T** (in that order) only when $\mathcal{D}_T \cup \mathcal{R}_T \subset \mathcal{D}_B$ and $B(T(x)) = T(B(x))$ for every $x \in \mathcal{D}_T$. It is implied by the existence of the right-hand side that $B(x) \in \mathcal{D}_T$ whenever $x \in \mathcal{D}_T$.

Equivalently, $\mathcal{D}_{B \circ T} = \mathcal{D}_T$ and $B \circ T \subset T \circ B$. A common case is when B is defined on all of $\mathcal{H}$, in which case the first condition (in both forms of the definition) is superfluous.

Note that if B commutes with T and T commutes with B then our definition puts strong conditions on domains and ranges. Specifically, $\mathcal{D}_B = \mathcal{D}_T$ and $\mathcal{R}_B \cup \mathcal{R}_T \subset \mathcal{D}_T$.

And whenever $\mathcal{D}_B = \mathcal{D}_T$, if B commutes with T then we do have symmetry: T commutes with B also.

Recall now the definition of a closed operator, and the results of Section **??**.

In our context, and using our identification of a function *as* its graph, T is closed when T is a closed subset of $\mathcal{H} \times \mathcal{H}$ with its natural inner product. This means that whenever sequence x_i, $i \in \mathbb{N}$, in $\mathcal{H}$ converges to a point $a \in \mathcal{H}$ and provided $T(x_i)$ converges to a point $b \in \mathcal{H}$ then $a \in \mathcal{D}_T$ and $T(a) = b$.

This condition is implied by continuity, but does not require continuity. The Closed Graph Theorem, Proposition **??**, states that when $f\colon X \to Y$ is linear and X and Y are Banach then f closed implies f continuous. But in our case that theorem applies only when $\mathcal{D}_T$ is a closed subset of the Hilbert space $\mathcal{H}$. This is allowed, but not the case of primary concern to us.

T is closed when T and its topological closure $\overline{T}$ in $\mathcal{H} \times \mathcal{H}$ coincide, and T is called closeable if $\overline{T}$ is a function. We saw in Corollary **??** that this will happen exactly when $(0, y) \in \overline{T}$ implies $y = 0$. In terms of $\mathcal{D}_T$, this condition means that whenever x_i converges to 0 in $\mathcal{D}_T$ then either $T(x_i)$ converges to 0 or $T(x_i)$ fails to converge at all.

In particular examples, a closed operator S is usually not given directly, but instead is the closure $\overline{T} = S$ of an operator T defined on smaller domain. $\mathcal{D}_T$ is then called a **core** of S.

1.1. ***Exercise***. *(i) If it is to be a core of closed Hilbert space operator S, it is necessary that subspace X of $\mathcal{D}_S$ be dense in $\mathcal{D}_S$. If S is bounded this is also sufficient.*

(ii) Assuming that there actually is a closeable unbounded operator with domain dense in $\mathcal{H}$ (we discuss several in later sections) show that the boundedness condition on S in (i) cannot be removed. (hint: In Exercise **??** *(ii) we saw that no unbounded closed operator T can be defined on all of $\mathcal{H}$. That means there is a vector x for which $T(y_i)$ fails to converge for every sequence y_i in $\mathcal{D}_T$ that converges to x. So let $\mathcal{D}_S = \mathbb{F}\, x \oplus \mathcal{D}_T$ and define S on $\mathcal{D}_S$ to be an extension of T.)*

(iii) Suppose T is closeable and $R \subset \overline{T}$. Then $\mathcal{D}_R$ is a core of $\overline{T}$ if every member x of $\mathcal{D}_T$ is a limit of some sequence y_i in $\mathcal{D}_R$ for which $R(y_i)$ converges.

(iv) If closed S is bounded below and has closed range $\mathcal{R}_S$, and if $S(X)$ is dense in $\mathcal{R}_S$ for dense subspace X of $\mathcal{D}_S$ then X is a core of S.

For unbounded T, if $\overline{T}$ is a function then $\mathcal{D}_{\overline{T}}$ contains every member a of $\mathcal{H}$ for which there is *any* sequence x_i in $\mathcal{D}_T$ converging to a with the property that $T(x_i)$ is also convergent. If this limit is b then $\overline{T}(a) = b$.

Suppose S is any extension of $\overline{T}$, and suppose $(a, b) \in S$.

If $a \in \overline{\mathcal{D}_T}$ then since $\mathcal{D}_T$ is dense in $\overline{\mathcal{D}_T}$ there is a sequence x_i from $\mathcal{D}_T$ with x_i converging to a. If $(a, b) \notin \overline{T}$ then it must be that $S(x_i) = T(x_i)$ fails to converge, and in fact there is no sequence y_i in $\mathcal{D}_T$ converging to a for which $T(y_i)$ converges to *anything*. So $b = S(a)$ has no connection to the values of T. And if $a \notin \overline{\mathcal{D}_T}$ then this is even more obviously true.

Extensions of T beyond $\overline{T}$ can be made "at random" (subject to linearity) but these extensions, even if they might be good for *something*, cannot be said to have anything to do with T. On the other hand, every point of $\overline{T}$ not already in T is connected to the values of T by a continuity condition at that new domain member, and there is only one possible way of doing this.

So $\overline{T}$ is the smallest closed extension of T, and the only one whose values are all connected by a continuity condition to the values of T itself.

It is important to recognize that if T is closeable there is no reason why $\mathcal{D}_{\overline{T}}$ should be closed. Generally it will not be.

In the following, we will consider functions defined on vector subspaces of a Hilbert space $\mathcal{H}$. We have certain requirements on a function T in the remainder of this section, and *if any these requirements are not met for some T we will be explicit about that.*

- $T\colon \mathcal{D}_T \to \mathcal{H}$ is linear on vector subspace $\mathcal{D}_T$ of Hilbert space $\mathcal{H}$.
- We ***require*** $\mathcal{D}_T$ to be ***dense*** in $\mathcal{H}$.
- We assume the field to be the complex numbers.
- We specifically ***do not*** require T to be bounded.

Generally, an operator satisfying these conditions is called an **unbounded operator on $\mathcal{H}$**.

It is an awkward phrase, as we do not exclude the possibility that such an operator is bounded, but it may not be, and many of the operators from important applications will not be. Also, the operator will not generally be defined *on* $\mathcal{H}$, but only on a proper dense subset.

For each $y \in \mathcal{H}$ define the function $A_y(\cdot) = \langle\, T(\cdot)\,,\, y\,\rangle\colon \mathcal{D}_T \to \mathbb{C}$.

A_y is linear on $\mathcal{D}_T$ and *if* it is bounded on $\mathcal{D}_T$ corresponds to inner product against a unique member $w_y \in \mathcal{H}$: viz.

$$A_y(\cdot) = \langle\, \cdot\,,\, w_y\,\rangle.$$

Since $\mathcal{D}_T$ is assumed dense in $\mathcal{H}$, w_y is the unique member of $\mathcal{H}$ that "works" for this y, and this uniqueness is one reason to require $\mathcal{D}_T$ to be dense in $\mathcal{H}$.

We define $T^\dagger(y) = w_y$ whenever A_y is a bounded functional on $\mathcal{D}_T$.

So $T^\dagger$ has its own domain, consisting of all those y for which the functional $A_y(\cdot) = \langle\, T(\cdot)\,,\, y\,\rangle$ is bounded.

The function $\mathbf{T}^\dagger\colon \mathcal{D}_{T^\dagger} \to \mathcal{H}$ defined by

$$\langle\, x\,,\, T^\dagger(y)\,\rangle = \langle\, T(x)\,,\, y\,\rangle \quad \forall x \in \mathcal{D}_T,\ y \in \mathcal{D}_{T^\dagger}$$

is called **the adjoint** of T. **Without further conditions we might not have $\mathcal{D}_{T^\dagger}$ dense in $\mathcal{H}$, and will provide an example illustrating this later.**

If S extends T (that is, if $T \subset S$) there is a relationship between $T^\dagger$ and $S^\dagger$.

1.2. ***Lemma***. *If S and T are unbounded operators on $\mathcal{H}$ and $T \subset S$ then $S^\dagger \subset T^\dagger$.*

Proof. Since $\mathcal{D}_T \subset \mathcal{D}_S$ and S agrees with T on $\mathcal{D}_T$, for each $y \in \mathcal{H}$ it is harder for $A_y(x) = \langle\, T(x)\,,\, y\,\rangle\ \forall x \in \mathcal{D}_T$ to be bounded than for $B_y(x) = \langle\, T(x)\,,\, y\,\rangle\ \forall x \in \mathcal{D}_S$ to be bounded. So $\mathcal{D}_{S^\dagger} \subset \mathcal{D}_{T^\dagger}$.

Now suppose $y \in \mathcal{D}_{S^\dagger}$. Then

$$\langle\, x\,,\, S^\dagger(y)\,\rangle = \langle\, S(x)\,,\, y\,\rangle \quad \forall x \in \mathcal{D}_S.$$

But $\mathcal{D}_T \subset \mathcal{D}_S$ and S agrees with T on $\mathcal{D}_T$ so

$$\langle\, x\,,\, S^\dagger(y)\,\rangle = \langle\, T(x)\,,\, y\,\rangle = A_y(x) \quad \forall x \in \mathcal{D}_T.$$

Since $T^\dagger(y)$ is the unique member of $\mathcal{H}$ that represents A_y on $\mathcal{D}_T$, we find $S^\dagger(y) = T^\dagger(y)$ for $y \in \mathcal{D}_{S^\dagger}$. □

1.3. ***Lemma***. *$T^\dagger$ is a closed operator for any unbounded operator T.*

Proof. Suppose x_i is a sequence in $\mathcal{D}_{T^\dagger}$ and x_i converges to a and $T^\dagger(x_i)$ converges to b. So

$$\langle\, x\,,\, T^\dagger(x_i)\,\rangle = \langle\, T(x)\,,\, x_i\,\rangle \quad \forall x \in \mathcal{D}_T.$$

The left side converges to $\langle\, x\,,\, b\,\rangle$ and the right side to $\langle\, T(x)\,,\, a\,\rangle$ for all $x \in \mathcal{D}_T$.

So we have: $\qquad \langle\, x\,,\, b\,\rangle = \langle\, T(x)\,,\, a\,\rangle \quad \forall x \in \mathcal{D}_T.$

That means $|\,\langle\, T(x)\,,\, a\,\rangle\,| \leq \|b\|\,\|x\|$ for all $x \in \mathcal{D}_T$ so $a \in \mathcal{D}_{T^\dagger}$. And the uniqueness condition mentioned earlier implies that $T^\dagger(a) = b$. □

1.4. ***Corollary***. *$T^\dagger$ is continuous exactly when $\mathcal{D}_{T^\dagger}$ is closed.*

Proof. By the last lemma $T^\dagger$ is closed so if $\mathcal{D}_{T^\dagger}$ is closed the closed graph theorem tells us that $T^\dagger$ is continuous.

On the other hand, suppose $T^\dagger$ is continuous and x_n is a sequence in $\mathcal{D}_{T^\dagger}$ converging to a point x. The sequence is bounded and $\|\, T^\dagger\,\| < \infty$ so there is a constant K for which $\|\, T^\dagger(x_n)\,\| < K$ for all n.

For each $w \in \mathcal{D}_T$ we find $|\,\langle\, T(w)\,,\, x_n\,\rangle\,| = |\,\langle\, w\,,\, T^\dagger(x_n)\,\rangle\,| \leq K\,\|\, w\,\|$. So by continuity of inner product we have $|\,\langle\, T(w)\,,\, x\,\rangle\,| \leq K\,\|\, w\,\|$ as well, which puts $x \in \mathcal{D}_{T^\dagger}$. □

1.5. ***Corollary***. *If $T^\dagger$ is bounded below (i.e. $T^\dagger$ has continuous inverse) then $\mathcal{R}_{T^\dagger}$ is closed.*

Proof. Suppose $T^\dagger(x_n)$ is Cauchy in $\mathcal{R}_{T^\dagger}$, converging to point $y \in \mathcal{H}$. Since $T^\dagger$ is bounded below x_n is Cauchy too, converging to some $x \in \mathcal{H}$.

Since $T^\dagger$ is closed $T^\dagger(x) = y \in \mathcal{R}_{T^\dagger}$. □

We define $\boldsymbol{J} \colon \boldsymbol{\mathcal{H}} \times \boldsymbol{\mathcal{H}} \to \boldsymbol{\mathcal{H}} \times \boldsymbol{\mathcal{H}}$ by

$$J(x, y) = (-y, x).$$

Note that J is an isometry and $J^2 = -I$ where I is the identity operator on $\mathcal{H} \times \mathcal{H}$ with product inner product

$$\langle\, (a, b)\,,\, (x, y)\,\rangle = \langle\, a\,,\, x\,\rangle + \langle\, b\,,\, y\,\rangle$$

Because J is an isometry on a complete space, if $A \subset \mathcal{H} \times \mathcal{H}$ is closed then so is $J(A)$. Obviously, two pairs (x, y) and (a, b) are orthogonal in $\mathcal{H} \times \mathcal{H}$ exactly when $J(x, y)$ and $J(a, b)$ are orthogonal.

If T is any linear operator and c a nonzero number, the operator $c\,T$ is normally regarded as the operator that sends x to $c\,T(x)$ and so the function $c\,T$ will contain the point $(\,x,\, c\,T(x)\,)$ for each $x \in \mathcal{D}_T$. But when T is regarded as a subset of $\mathcal{H} \times \mathcal{H}$, $c\,T$ means the set of all $(\,c\,x,\, c\,T(x)\,)$ for $x \in \mathcal{D}_T$, and by linearity this is just T.

Keep an eye out for this: in the equation $J^2(T) = -T = T$ it is this second meaning that is intended. $J^2(x,y) = (-x,-y)$ for each $(x,y) \in T$ but the *sets* $J^2(T)$ and T coincide when T is linear.

1.6. ***Lemma***. *When T is a closed operator.*

Then $J(T^\dagger) = T^\perp$ and $\mathcal{H} \times \mathcal{H} = T \oplus T^\perp = T \oplus J(T^\dagger)$

where these direct sums are orthogonal direct sums.

Proof. Suppose $(y, T^\dagger(y)) \in T^\dagger$. Then for every $x \in \mathcal{D}_T$ we find

$$0 = \langle\, x\,,\, T^\dagger(y)\,\rangle \;-\; \langle\, T(x)\,,\, y\,\rangle = \langle\, J(x,T(x))\,,\,(y,T^\dagger(y))\,\rangle.$$

So every member of $T^\dagger$ is orthogonal to every member $J(T)$ and, of course, we then have every member of $J(T^\dagger)$ orthogonal to every member of T as well.

On the other hand, suppose $(a,b) \in T^\perp$. Then for every $x \in \mathcal{D}_T$ we have

$$0 = \langle\, x\,,\, a\,\rangle + \langle\, T(x)\,,\, b\,\rangle$$

which implies that $\langle\, T(\cdot)\,,\, b\,\rangle$ is bounded on $\mathcal{D}_T$ so $b \in \mathcal{D}_{T^\dagger}$. By the uniqueness condition implied by the density of $\mathcal{D}_T$ we then have $a = -T^\dagger(b)$ and $(a,b) \in J(T^\dagger)$.

Our conclusion here is that $J(T^\dagger) = T^\perp$, and the remaining statements of the lemma are immediate. □

1.7. ***Proposition***. *When T is a closeable operator then $\overline{T}^\dagger = T^\dagger$ and $\mathcal{D}_{T^\dagger}$ is dense in $\mathcal{H}$.*

Proof. Since $\overline{T}$ extends T we know that $\mathcal{D}_{\overline{T}^\dagger} \subset \mathcal{D}_{T^\dagger}$ and that $\overline{T}^\dagger$ agrees with $T^\dagger$ on $\mathcal{D}_{\overline{T}^\dagger}$. We will now show that $\mathcal{D}_{T^\dagger} - \mathcal{D}_{\overline{T}^\dagger}$ must be empty, so that $\overline{T}^\dagger = T^\dagger$.

Suppose $y \in \mathcal{D}_{T^\dagger} - \mathcal{D}_{\overline{T}^\dagger}$.

The operator norm of $\langle\, \overline{T}(\cdot)\,,\, y\,\rangle = \langle\, T(\cdot)\,,\, y\,\rangle$ is bounded by some number k on $\mathcal{D}_T$ but $\langle\, \overline{T}(\cdot)\,,\, y\,\rangle$ is unbounded on $\mathcal{D}_{\overline{T}}$.

So there must be a point $(x, \overline{T}(x)) \in \overline{T}$ for which x is in the unit sphere in $\mathcal{D}_{\overline{T}}$ and $|\,\langle\, \overline{T}(x)\,,\, y\,\rangle\,| > k+1$.

This x cannot be in $\mathcal{D}_T$, but there is a sequence x_i in the unit sphere in $\mathcal{D}_T$ converging to x and for which $T(x_i)$ converges to $\overline{T}(x)$. But then

$$|\,\langle\, T(x_i)\,,\, y\,\rangle\,| \le k < k+1 < |\,\langle\, \overline{T}(x)\,,\, y\,\rangle\,|$$

contradicting continuity of inner product.

So no such y can exist and therefore $\overline{T}^\dagger = T^\dagger$.

We will now show that in case T is closeable that $\mathcal{D}_{T^\dagger} = \mathcal{D}_{\overline{T}^\dagger}$ is dense in $\mathcal{H}$.

We will suppose, without loss, that T itself is closed: that is, T is a closed subspace of the Hilbert space $\mathcal{H} \times \mathcal{H}$.

We now suppose that $a \in (\mathcal{D}_{T^\dagger})^\perp$. Our goal here is to conclude that $a = 0$ so $(\mathcal{D}_{T^\dagger})^\perp = \{\,0\,\}$ and we could conclude that $\mathcal{D}_{T^\dagger}$ is dense.

We do know that for every $y \in \mathcal{D}_{T^\dagger}$ we have

$$0 = \langle\, -T^\dagger(y)\,,\, 0\,\rangle + \langle\, a\,,\, y\,\rangle = \langle\,(0,a)\,,\,(-T^\dagger(y),y)\,\rangle = \langle\,(0,a)\,,\, J(y,T^\dagger(y))\,\rangle.$$

That means $(0, a) \in T = \big(J(T^\dagger)\big)^\perp$ by Lemma 1.6 (remember, we are assuming here that $T = \overline{T}$) and since T is a linear function we must have $a = 0$ as required. □

1.8. ***Proposition***. *For unbounded operator T if $\mathcal{D}_{T^\dagger}$ is dense then T is closeable and $\overline{T} = T^{\dagger\dagger}$.*

PROOF. Suppose $(0, b) \in \overline{T}$. So there is a sequence x_i of members of $\mathcal{D}_T$ converging to 0 for which $T(x_i)$ converges to b. Then for each $y \in \mathcal{D}_{T^\dagger}$ we have

$$\langle T(x_i)\,,\, y\,\rangle = \langle\, x_i\,,\, T^\dagger(y)\,\rangle$$

and the right side converges to 0. If $\mathcal{D}_{T^\dagger}$ is dense, continuity of inner product requires b to be 0 and so $\overline{T}$ is a function and T is closeable.

Recall the notation in the proof of Lemma 1.6 and Proposition 1.7.

If $\mathcal{D}_{T^\dagger}$ is dense

$$\mathcal{H} \times \mathcal{H} = T^\dagger \oplus (T^\dagger)^\perp = T^\dagger \oplus J(T^{\dagger\dagger}) = \big(J(\overline{T})\big)^\perp \oplus J(T^{\dagger\dagger})$$

where all direct sums are orthogonal direct sums.

So $(\overline{T})^\perp = \big(T^{\dagger\dagger}\big)^\perp$ and it follows that $\overline{T} = T^{\dagger\dagger}$. □

1.9. ***Exercise***. *(i)* $(\,\mathcal{R}_T\,)^\perp = Ker\,\big(T^\dagger\big)$.

(ii) $(\,\mathcal{R}_{T^\dagger}\,)^\perp \supset Ker\,(T)$. *And if T is closed then* $(\,\mathcal{R}_{T^\dagger}\,)^\perp = Ker\,(T)$.

1.10. ***Corollary***. *Suppose T is closeable. T is one-to-one if and only if $\mathcal{R}_{T^\dagger}$ is dense in $\mathcal{H}$.*

PROOF. Rephrase Exercise 1.9. □

1.11. ***Corollary***. *If $\mathcal{D}_T = \mathcal{H}$ and $\mathcal{D}_{T^\dagger}$ is dense in $\mathcal{H}$ then T is continuous.*

PROOF. If $\mathcal{D}_{T^\dagger}$ is dense then $\overline{T} = T^{\dagger\dagger}$. Since T is already defined on $\mathcal{H}$ we have $\overline{T} = T$ so T is closed. Now Corollary 1.4 tells us that $T = T^{\dagger\dagger}$ is continuous. □

1.12. ***Lemma***. *Suppose S is one-to-one and $\mathcal{R}_S$ is dense in $\mathcal{H}$. So both S and S^{-1} are unbounded operators. Then $S^\dagger$ is one-to-one and $\big(S^\dagger\big)^{-1} = \big(S^{-1}\big)^\dagger$.*

PROOF. By Exercise 1.9 (i) $Ker(S^\dagger)$ is trivial so $S^\dagger$ is one-to-one.

$$\begin{aligned}
(a,b) \in \big(S^\dagger\big)^{-1} &\iff (b,a) \in S^\dagger \iff S^\dagger(b) = a \\
&\iff \forall x \in \mathcal{D}_S \quad \langle\, S(x)\,,\, b\rangle = \langle\, x\,,\, a\rangle \\
&\iff \forall y \in \mathcal{R}_S \quad \langle\, y\,,\, b\rangle = \langle\, S^{-1}(y)\,,\, a\rangle \\
&\iff b = \big(S^{-1}\big)^\dagger(a) \iff (a,b) \in \big(S^{-1}\big)^\dagger .
\end{aligned}$$

□

1.13. ***Lemma***. *$\mathcal{R}_{S^\dagger} = \mathcal{H}$ if and only if S is bounded below.*

PROOF. Assume $\mathcal{R}_{S^\dagger} = \mathcal{H}$ but S is not bounded below.

Select sequence x_n in the domain of S with $\| x_n \| \to \infty$ but $S(x_n) \to 0$. Consider the family of continuous functionals ϕ_n given by $\phi_n(w) = \langle w , x_n \rangle$ for each n. Note that $\| \phi_n \| = \| x_n \| \to \infty$.

Since $S^\dagger$ is onto $\mathcal{H}$ every $w \in \mathcal{H}$ is of the form $S^\dagger(y)$ for some $y \in \mathcal{D}_{S^\dagger}$. Then

$$\phi_n(w) = \langle w , x_n \rangle = \langle S^\dagger(y) , x_n \rangle = \langle y , S(x_n) \rangle \to 0.$$

So the set $\{ \phi_n(w) \mid n \in \mathbb{N} \}$ is bounded for every $w \in \mathcal{H}$. So by the Banach-Steinhaus Theorem there is a constant M for which $\| \phi_n \| \leq M$ for every n. This contradicts our earlier observation about these operator norms. So S is bounded below.

We now suppose S is bounded below.

Then $S^{-1} \colon \mathcal{R}_S \to \mathcal{D}_S$ exists and is continuous.

For every $w \in \mathcal{H}$ the functional $\phi_w(\cdot) = \langle S^{-1}(\cdot) , w \rangle$ is continuous on $\mathcal{R}_S$ and so can be extended to a continuous functional on all of $\mathcal{H}$. Any such can be represented as inner product against a member z of $\mathcal{H}$, so

$$\langle S^{-1}(x) , w \rangle = \langle x , z \rangle \quad \forall x \in \mathcal{R}_S.$$

So if $x = S(y)$ we have

$$\langle y , w \rangle = \langle S(y) , z \rangle \quad \forall y \in \mathcal{D}_S.$$

That means $z \in \mathcal{D}_{S^\dagger}$ and $S^\dagger(z) = w$. So arbitrarily chosen w is in $\mathcal{R}_{S^\dagger}$. □

1.14. ***Corollary***. *Suppose S is closed.*
$\mathcal{R}_S = \mathcal{H}$ if and only if $S^\dagger$ is bounded below.

PROOF. Since S is closed, $S^{\dagger\dagger} = S$ and we can apply the last lemma, replacing S with $S^\dagger$. □

1.15. ***Theorem***. *Suppose S is closed.*
$\mathcal{R}_S = \mathcal{H}$ and S is bounded below if and only if
$\mathcal{R}_{S^\dagger} = \mathcal{H}$ and $S^\dagger$ is bounded below.

PROOF. This follows from Lemma 1.13 and its corollary. □

2. Spectrum and Resolvent

For unbounded operator T on $\mathcal{H}$ and complex number α, if $T - \alpha I$ has trivial kernel then it has an inverse function called the **resolvent for T and $\boldsymbol{\alpha}$**

$$\mathbf{R}_{\boldsymbol{\alpha}}(\mathbf{T}) = (T - \alpha I)^{-1} \colon (T - \alpha I)(\mathcal{D}_T) \to \mathcal{D}_T.$$

$T - \alpha I$ is bounded below if and only if $R_\alpha(T)$ is bounded on its domain, which is equivalent to continuity of this inverse map. In particular,

$$\| (T - \alpha I)(x) \| \geq c \| x \| \ \forall x \in \mathcal{D}_T \text{ if and only if } \| R_\alpha(y) \| \leq \frac{1}{c} \| y \| \ \forall y \in \mathcal{R}_{T - \alpha I},$$

where in this statement c is a positive constant.

If $R_\alpha(T)$ is continuous with dense domain α is called a **regular value for T**. The set of all regular values is called the **resolvent set**, $\boldsymbol{\rho}(\mathbf{T})$, and the set of complex numbers *not* in the resolvent set is called the **spectrum**, $\boldsymbol{\sigma}(\mathbf{T})$.

Complex numbers can wind up in the spectrum, potentially, for three reasons.

It might be that α is an eigenvalue for T, so $T - \alpha I$ has no inverse at all. The collection of eigenvalues is called the **point spectrum.** The point spectrum is denoted $\boldsymbol{\sigma}_{\mathbf{p}}(\mathbf{T})$. There is no distinction made among members of the point spectrum for which $T - \alpha I$ has dense range and those for which the range is not dense.[1]

If α is *not* an eigenvalue and $T - \alpha I$ has dense range but $T - \alpha I$ is *not* bounded below, then $R_\alpha(T)$ still exists as an unbounded operator and these α comprise the **continuous spectrum** denoted $\boldsymbol{\sigma}_{\mathbf{c}}(\mathbf{T})$.

And members α of the spectrum which are *not* eigenvalues but for which $T - \alpha I$ does *not* have dense range, whether or not $T - \alpha I$ is bounded below, comprise the **residual spectrum** denoted $\boldsymbol{\sigma}_{\mathbf{r}}(\mathbf{T})$.

As a final piece of vocabulary we gather together all of σ_p and σ_c and possibly some of the members of σ_r to form the **approximate point spectrum** denoted $\boldsymbol{\sigma}_{\mathbf{ap}}(\mathbf{T})$. This set consists of those α for which there is a sequence x_n of unit vectors in $\mathcal{D}_T$ with $\| (T - \alpha I)(x_n) \| \to 0$. It may be convenient to find a sequence x_n of vectors in $\mathcal{D}_T$ for which $\| x_n \| \to \infty$ and for which $\| (T - \alpha I)(x_n) \| \to 0$, and this condition can, equivalently, serve to define the approximate point spectrum.

2.1. ***Lemma***. *$\alpha \in \sigma_{ap}(T)$ if and only if there is a sequence x_n of unit vectors in $\mathcal{D}_T$ for which*

$$\langle T(x_n) - \alpha x_n , x_n \rangle \to 0 \text{ and } \langle T(x_n) , x_n \rangle \to \alpha \text{ and } \langle T(x_n) , T(x_n) \rangle \to \alpha \overline{\alpha}.$$

PROOF. Suppose $\alpha \in \sigma_{ap}$. Then there is a sequence x_n of unit vectors in $\mathcal{D}_T$ with $\| T(x_n) - \alpha x_n \| \to 0$. But then

$$| \langle T(x_n) - \alpha x_n , x_n \rangle | \leq \| T(x_n) - \alpha x_n \| \| x_n \| = \| T(x_n) - \alpha x_n \| \to 0.$$

So $\langle T(x_n) , x_n \rangle - \langle \alpha x_n , x_n \rangle = \langle T(x_n) , x_n \rangle - \alpha \to 0$.

Expand $\langle T(x_n) - \alpha x_n , T(x_n) - \alpha x_n \rangle$ to obtain the remaining limits and the converse implication. □

$\sigma_{ap}(T)$ consists of exactly those α for which $T - \alpha I$ is *not* bounded below.

So $\sigma_r(T) - \sigma_{ap}(T)$ corresponds to those complex numbers α for which $T - \alpha I$ *is* bounded below but for which $\mathcal{R}_{T - \alpha I}$ *is not* dense.

If T is fixed during a discussion, repeated reference to it might be suppressed to clean up the notation. So the resolvent R_α exists and is bounded on the resolvent set ρ, and the spectrum $\sigma = \mathbb{C} - \rho$ can be written as:

the ***disjoint* union** $\sigma = \sigma_p \cup \sigma_c \cup \sigma_r$ and as the **union** $\sigma = \sigma_{ap} \cup \sigma_r$.

[1]Different authors chop the spectrum up in various ways and with various names, and we don't propose to analyze all the different vocabularies. Descriptors for pieces of the spectrum include: discrete, pure point, peripheral, essential, absolutely continuous, singular and compression, in addition to our vocabulary. The reader of a given text must winkle out the usage in context.

2.2. ***Lemma***. *If T is an unbounded operator and $T \subset S \subset \overline{T}$ then*

$$\sigma_r\,(S) \subset \sigma_r(T) \text{ and } \sigma_{ap}\,(S) = \sigma_{ap}(T) \text{ so } \sigma\,(S) \subset \sigma(T).$$

While S could have more eigenvalues than T, it acquires them from $\sigma_c(T)$ or $\sigma_{ap}(T) \cap \sigma_r(T)$.

Proof. If $(\,S - \alpha\,I\,)\,(\mathcal{D}_S)$ is not dense then its subset $(\,T - \alpha\,I\,)\,(\mathcal{D}_T)$ cannot be, so clearly $\sigma_r\,(S) \subset \sigma_r(T)$.

It is also obvious that $\sigma_{ap}\,(T) \subset \sigma_{ap}(S)$, since any sequence of unit vectors x_n drawn from $\mathcal{D}_T$ for which $(\,T - \alpha\,I\,)(x_n) \to 0$ will serve as well to place $\alpha \in \sigma_{ap}(S)$.

Now suppose x_n is a sequence in $\mathcal{D}_S$ for which $(\,S - \alpha\,I\,)(x_n) \to 0$. Since $\mathcal{D}_S \subset \mathcal{D}_{\overline{T}}$ for each n there is a unit vector y_n from $\mathcal{D}_T$ for which both $\|\,x_n - y_n\,\| < \frac{1}{n}$ and $\|\,S(x_n) - T(y_n)\,\| < \frac{1}{n}$. But then

$$\begin{aligned}0 \leq |\,\|\,(\,S - \alpha\,I\,)(x_n)\,\| - \|\,(\,T - \alpha\,I\,)(y_n)\,\| \\ \leq \|\,S(x_n) - \alpha\,x_n - T(y_n) + \alpha\,y_n\,\| \\ \leq \|\,S(x_n) - T(y_n)\,\| + \alpha\,\|\,y_n - x_n\,\| \to 0.\end{aligned}$$

By assumption $(\,S - \alpha\,I\,)(x_n) \to 0$ so $(\,T - \alpha\,I\,)(y_n) \to 0$ as well so $\alpha \in \sigma_{ap}(T)$. □

2.3. ***Exercise***. *Find an example of unbounded operators T and W with $T \subset \overline{T} \subset W$ and for which (i) $\sigma(T) \neq \sigma(W)$ and $\sigma(T) \subset \sigma(W)$. (ii) Find another example with $\sigma(T) \not\subset \sigma(W)$ and $\sigma(W) \not\subset \sigma(T)$.*

2.4. ***Lemma***. *Suppose T is closed and operator $T - \alpha\,I$ is bounded below for some number α. This is equivalent to continuity of the resolvent function for T and α.*
Then the range of $T - \alpha\,I$ is closed. So if it is dense in $\mathcal{H}$ it must be all of $\mathcal{H}$.

Proof. Suppose $(T - \alpha\,I)(x_n) \to y$. Since $T - \alpha\,I$ is bounded below x_n is Cauchy and so converges to some $x \in \mathcal{H}$. That means $T(x_n) = \alpha\,x_n + y$ is a sequence in $\mathcal{R}_T$ which converges to $\alpha\,x + y$, and since T is closed $x \in \mathcal{D}_T$ and $T(x) = \alpha\,x + y$. So $(T - \alpha\,I)(x) = y$ is in the range of $T - \alpha\,I$. □

2.5. ***Exercise***. *For operator T the residual spectrum can be decomposed as*

$$\sigma_r = (\,\sigma_r - \sigma_{ap}\,) \cup (\,\sigma_r \cap \sigma_{ap}\,).$$

(i) If $\alpha \in \sigma_r - \sigma_{ap}$, the resolvent R_α is continuous. If $\alpha \in \sigma_r \cap \sigma_{ap}$ the resolvent is not continuous.

(ii) Whenever $\alpha \in \sigma_r$ the domain of the resolvent R_α, $\mathcal{R}_{T-\alpha\,I}$, is not dense in $\mathcal{H}$. In particular

$$(\,\mathcal{R}_{T-\alpha\,I}\,)^\perp = Ker\left(T^\dagger - \overline{\alpha}\,I\right) \neq \{\,0\,\}.$$

If T is closed we have $\mathcal{R}_{T-\alpha\,I}$ closed, so $\mathcal{R}_{T-\alpha\,I} = Ker\left(T^\dagger - \overline{\alpha}\,I\right)^\perp \neq \mathcal{H}$.

Whether T is closed or not, $\overline{\mathcal{R}_{T-\alpha\,I}}$ is the orthogonal complement of the eigenspace of $T^\dagger$ for eigenvalue $\overline{\alpha}$, and this eigenspace is nontrivial.

2.6. ***Lemma***. *If T is an unbounded operator and $T - \alpha I$ is bounded below for some number α then $T - \beta I$ is bounded below for all β in some disk of positive radius around α.*

Specifically, if $\| R_\alpha(T) \| \le k$ and $| \beta - \alpha | < \frac{1}{k}$ then

$$\| R_\beta(T) \| \le \left(\frac{1}{k} - | \beta - \alpha | \right)^{-1}.$$

Proof. If $\| (T - \alpha I)(x) \| \ge \varepsilon \| x \|$ for some positive ε and number α and operator T, and if $\eta \in \mathbb{C}$ with $|\eta| < \varepsilon$ then

$$\begin{aligned} \| (T - \alpha I - \eta I)(x) \| &\ge \| (T - \alpha I)(x) \| - \| \eta x \| \\ &\ge \varepsilon \| x \| - |\eta| \| x \| = (\varepsilon - |\eta|) \| x \|. \end{aligned}$$

□

This lemma tells us that complex numbers sufficiently near a member of the resolvent set are themselves in the resolvent set *provided that the domain of the corresponding resolvent function is dense.*

2.7. ***Lemma***. *For unbounded operator T, if $\rho = \rho(T) \ne \varnothing$ then T is closed.*

Proof. Suppose ρ is nonempty and $\alpha \in \rho$. Suppose further that $(x_n, T(x_n))$ is convergent to a point (a, b) in $\mathcal{H} \times \mathcal{H}$. Then R_α is continuous so

$$\begin{aligned} R_\alpha(b - \alpha a) &= \lim_{n\to\infty} R_\alpha(T(x_n) - \alpha x_n) \\ &= \lim_{n\to\infty} (T - \alpha I)^{-1} (T - \alpha I)(x_n) = \lim_{n\to\infty} x_n = a. \end{aligned}$$

Since the range of R_α is $\mathcal{D}_T$, this means $a \in \mathcal{D}_T$. And now

$$b - \alpha a = (T - \alpha I)(T - \alpha I)^{-1}(b - \alpha a) = (T - \alpha I)(a) = T(a) - \alpha a$$

So we find that $T(a) = b$ and therefore T is closed. □

Suppose α is in the resolvent set for operator T. We have just found that R_α has domain $\mathcal{H}$. We know that R_β is continuous for β near to α but we don't (yet) know if the domain of a nearby R_β is dense—and therefore *also* $\mathcal{H}$.

If $\| R_\alpha \| = k$ define for complex β with $| \beta - \alpha | < \frac{1}{k}$ the expression

$$S_\beta = \sum_{n=0}^{\infty} (\beta - \alpha)^n R_\alpha^{n+1}.$$

The sequence of partial sums $P_j = \sum_{n=0}^{j} (\beta - \alpha)^n R_\alpha^{n+1}$ is Cauchy in operator norm and the continuous operators defined on all of $\mathcal{H}$ form a Banach space so the series does converge to a bounded operator defined, as is R_α, on all of $\mathcal{H}$.

$$
\begin{aligned}
(T-\beta I)P_j &= (T-\alpha I-(\beta-\alpha)I)P_j = (T-\alpha I)P_j-(\beta-\alpha)P_j \\
&= (T-\alpha I)\left(\sum_{n=0}^{j}(\beta-\alpha)^n R_\alpha^{n+1}\right)-(\beta-\alpha)\left(\sum_{n=0}^{j}(\beta-\alpha)^n R_\alpha^{n+1}\right) \\
&= I+\left(\sum_{n=1}^{j}(\beta-\alpha)^n R_\alpha^{n}\right)-\left(\sum_{n=0}^{j}(\beta-\alpha)^{n+1} R_\alpha^{n+1}\right) \\
&= I-(\beta-\alpha)^{j+1}R_\alpha^{j+1}.
\end{aligned}
$$

The last term converges to 0 in operator norm and we conclude that $(T-\beta I)P_j(x)$ converges to x for every $x \in \mathcal{H}$. Since the range of $T-\beta I$ is closed (we are assuming here that $\rho(T)$ is nonempty so T is closed) that range must be all of $\mathcal{H}$. So the domain of R_β is all of $\mathcal{H}$.

A similar argument shows that $P_j(T-\beta I)(x) \to x$ for each $x \in \mathcal{D}_T$, and it also converges to $S_\beta(T-\beta I)(x)$.

Putting these two together yields $S_\beta = R_\beta$, a series representation for the resolvent function for β in a neighborhood of any α in the resolvent set.

2.8. ***Proposition***. *(i) The resolvent set for any unbounded operator T is open.*

(ii) The spectrum of any unbounded operator T is closed.

(iii) The domain of R_α is $\mathcal{H}$ (not just dense in $\mathcal{H}$) for every $\alpha \in \rho(T)$.

(iv) If $\alpha \in \rho(T)$ and $\|R_\alpha\| = k$ and $\beta \in \mathbb{C}$ with $|\beta-\alpha| < \frac{1}{k}$ then $\beta \in \rho(T)$ and the following series representation is convergent in operator norm:

$$R_\beta = \sum_{n=0}^{\infty}(\beta-\alpha)^n R_\alpha^{n+1}.$$

Proof. If $\rho(T) = \varnothing$ there is nothing to prove. The case $\rho(T) \neq \varnothing$ is dealt with in the preceding remarks. □

When the resolvent set for an operator T is nonempty, there are several identities involving the resolvent that are useful and we develop them now.

2.9. ***Proposition***. *Suppose S and T are unbounded operators with nonempty resolvent sets. Suppose $\alpha, \beta \in \rho(T)$ and $\gamma \in \rho(T) \cap \rho(S)$.*

(i) Operator V commutes with T if and only if $R_\alpha(T)$ commutes with V.

(ii) $R_\alpha(T) - R_\beta(T) = (\alpha-\beta)\, R_\alpha(T)\, R_\beta(T)$.

(iii) $R_\gamma(T) - R_\gamma(S) = R_\gamma(T)\,(S-T)\,R_\gamma(S)$ when $\mathcal{D}_S \subset \mathcal{D}_T$.

Proof. (i) Suppose V commutes with T. Then both $\mathcal{D}_T$ and $\mathcal{R}_T$ are in $\mathcal{D}_V$ and for every $x \in \mathcal{D}_T$ we have $V(T(x)) = T(V(x))$. It is implied by the existence of the right-hand side that $V(x) \in \mathcal{D}_T$ whenever $x \in \mathcal{D}_T$.

We need to show that this implies that R_α commutes with V. Since $\mathcal{D}_{R_\alpha} = \mathcal{H}$ we have both domain and range of V in the domain of R_α. We need to show that $R_\alpha(V(x)) = V(R_\alpha(x))$ for all $x \in \mathcal{D}_V$. We do have the right side of this equation defined, since the range of R_α is $\mathcal{D}_T$ which is contained in $\mathcal{D}_V$ by assumption. Since $T - \alpha I$ is onto $\mathcal{H}$ there is a $y \in \mathcal{D}_T$ for which $T(y) - \alpha y = x$. Then

$$\begin{aligned} V(R_\alpha(x)) &= V(R_\alpha(T(y) - \alpha y)) = V(y) = R_\alpha(T - \alpha I)V(y) \\ &= R_\alpha(T(V(y)) - \alpha V(y)) = R_\alpha(V(T(y)) - V(\alpha y)) = R_\alpha(V(x)). \end{aligned}$$

So we have shown that if V commutes with T then $R_\alpha(T)$ commutes with V.

For the converse implication, suppose $R_\alpha(V(x)) \neq V(R_\alpha(x))$ for some $x \in \mathcal{D}_V$. Revisiting the last calculation above in reverse order, it must fail somewhere. There are only three places in the chain of equalities that this might occur. First, it may be that $T(y) \notin \mathcal{D}_V$, so V does not commute with T because $\mathcal{R}_T \not\subset \mathcal{D}_V$. But if $T(y) \in \mathcal{D}_V$, it might be that $T(V(y)) \neq V(T(y))$, and again V does not commute with T. Finally, it could be that $R_\alpha(x) \notin \mathcal{D}_V$. But the range of R_α is $\mathcal{D}_T$ so $\mathcal{D}_T \not\subset \mathcal{D}_V$ and, again, V does not commute with T.

(ii) $(T - \beta I)R_\beta(T)$ is the identity on $\mathcal{H}$ while $R_\alpha(T)(T - \alpha I)$ is the identity on $\mathcal{D}_T$.

$$\begin{aligned} R_\alpha(T) - R_\beta(T) &= R_\alpha(T)(T - \beta I)R_\beta(T) - R_\alpha(T)(T - \alpha I)R_\beta(T) \\ &= R_\alpha(T)(T - \beta I - T + \alpha I)R_\beta(T) = (\alpha - \beta)\, R_\alpha(T)\, R_\beta(T). \end{aligned}$$

(iii) Similarly to the calculation above, and using $\mathcal{D}_S \subset \mathcal{D}_T$, we have

$$\begin{aligned} R_\gamma(T) - R_\gamma(S) &= R_\gamma(T)(S - \gamma I)R_\gamma(S) - R_\gamma(T)(T - \gamma I)R_\gamma(S) \\ &= R_\gamma(T)(S - \gamma I - T + \gamma I)R_\gamma(S) = R_\gamma(T)(S - T)R_\gamma(S). \end{aligned}$$

□

Item (ii) of this proposition is generally referred to as **the First Resolvent Identity** while (iii) is called **the Second Resolvent Identity.** The First Resolvent Identity implies that $R_\alpha(T)$ and $R_\beta(T)$ commute whenever $\alpha, \beta \in \rho(T)$.

3. Symmetric Operators

In this section, as in the last, we work with operators defined on a dense vector subspace of a complex Hilbert space $\mathcal{H}$ unless explicitly stated to the contrary.

We call an unbounded operator T as above **symmetric** if $T \subset T^\dagger$: in other words, if $T^\dagger$ is an extension of T. Linear T is symmetric exactly when $T^\dagger(x)$ is defined for every $x \in \mathcal{D}_T$ and $T(x) = T^\dagger(x)$.

So T symmetric means that

$$\langle T(x)\,,\, y \rangle = \langle x\,,\, T(y) \rangle \quad \forall\, x, y \in \mathcal{D}_T.$$

The argument of Lemma **??** needs no modification for unbounded operators.

$$T \text{ is symmetric} \Leftrightarrow \langle T(x)\,,\, x \rangle = \langle x\,,\, T(x) \rangle \quad \forall\, x \in \mathcal{D}_T$$

and then of course we have the equivalent condition

$$T \text{ is symmetric} \Leftrightarrow \langle T(x)\,,\, x \rangle \ \text{ is real} \quad \forall\, x \in \mathcal{D}_T.$$

3.1. ***Proposition***. *If T is symmetric, the approximate point spectrum σ_{ap} of T is contained in $\mathbb{R}$.*

So if α is non-real and in the spectrum of T then the resolvent function R_α is continuous but fails to have dense domain: $\mathcal{R}_{T-\alpha I}$ cannot be dense in $\mathcal{H}$ for any such α.

Proof. Suppose $\alpha \in \sigma_{ap}$. Then there is a sequence x_n of unit vectors in $\mathcal{D}_T$ with $\| T(x_n) - \alpha x_n \| \to 0$. By Lemma 2.1 we have $\langle T(x_n), x_n \rangle \to \alpha$.

Symmetry now requires α to be real. □

See Proposition 3.4 for the next step in this direction.

Since $T^\dagger$ is always closed and $T^\dagger$ extends symmetric T, every symmetric operator is closeable.

If symmetric T is bounded on $\mathcal{D}_T$ then it could be extended in a unique way to a continuous operator $\overline{T}$ defined on all of $\mathcal{H}$. In that case, since $T^\dagger$ is closed we have $T^\dagger = \overline{T}$ and then $\overline{T} = T^{\dagger\dagger} = \overline{T}^\dagger$ so $\overline{T}$ is its own adjoint. This is the ordinary adjoint for bounded operators, and the symmetry condition just means that this unique extension of T to all of $\mathcal{H}$ is self-adjoint.

Bounded or not, the domain of $T^\dagger$ for symmetric T will often be larger than the domain of T.

3.2. ***Lemma***. *(i) A symmetric operator is always closeable.*
(ii) If T is symmetric and $\mathcal{D}_{\overline{T}} = \mathcal{H}$ (so $\overline{T} = T^\dagger$) then T is bounded.

Proof. See the preceding remarks for (i). Case (ii) follows Corollary 1.11 or from the preceding remarks and the closed graph theorem directly. □

Item (ii) of Lemma 3.2 is called **The Hellinger-Toeplitz Theorem.**

So if we know that symmetric T is *not* bounded, then we know that the domain of $T^\dagger$ *cannot* be all of $\mathcal{H}$: the Hellinger-Toeplitz Theorem tells us there is no getting away (in cases of crucial importance) from consideration of operators defined on only part of $\mathcal{H}$.

3.3. ***Lemma***. *Suppose S is symmetric and one-to-one.*
If $\mathcal{R}_S = \mathcal{D}_{S^{-1}}$ is dense in $\mathcal{H}$ then S^{-1} is symmetric too.

Proof. The domain of S^{-1} is $\mathcal{R}_S$.

Suppose $g = S(x)$ and $f = S(y)$ are in $\mathcal{D}_{S^{-1}}$. Then

$$\langle S^{-1}(g), f \rangle = \langle x, S(y) \rangle = \langle S(x), y \rangle = \langle g, S^{-1}(f) \rangle.$$

□

A symmetric T *might* have the same domain as $T^\dagger$, *and it is only to these unbounded operators that some of our most important theorems apply.*

If $T = T^\dagger$ we say that the unbounded operator T is **self-adjoint**. Self-adjoint operators are, of course, closed. If a self-adjoint operator (like any symmetric operator) has any eigenvalues at all they must be real.

3.4. ***Proposition***. *Suppose T is self-adjoint.*
If $\mathcal{R}_{T-\alpha I} = (T - \alpha I)(\mathcal{D}_T)$ is not dense in $\mathcal{H}$
then α is a real eigenvalue of T.
Self-adjoint operators have no residual spectrum.

PROOF. Suppose $A = \mathcal{R}_{T-\alpha I}$ is not dense in $\mathcal{H}$. Select nonzero $x \in A^{\perp}$.

So $\forall w \in \mathcal{D}_T$ we have (since T is self-adjoint)

$$0 = \langle (T - \alpha I)(w), x \rangle = \langle T(w), x \rangle - \langle \alpha w, x \rangle.$$

So $\langle T(w), x \rangle = \langle \alpha w, x \rangle$ for all $\forall w \in \mathcal{D}_T$, so the functional $\langle T(\cdot), x \rangle$ is bounded on $\mathcal{D}_T$. That means x is in the domain of $T^{\dagger}$, assumed to be equal to T. We can now carry the calculation above a step further:

$$0 = \langle (T - \alpha I)(w), x \rangle = \langle T(w), x \rangle - \langle \alpha w, x \rangle = \langle w, T(x) \rangle - \langle w, \overline{\alpha} x \rangle.$$

Since $\mathcal{D}_T$ is dense in $\mathcal{H}$ this means $T(x) = \overline{\alpha} x$. But T can have only real eigenvalues so α is real. □

3.5. ***Corollary***. *Suppose T is self-adjoint.*
The spectrum σ of T is contained in $\mathbb{R}$ and
$\sigma = \sigma_p \cup \sigma_c$.

PROOF. By Proposition 3.1 the resolvent function is continuous off the real numbers for every symmetric T. For self-adjoint operators, which are closed, Proposition 3.4 and Lemma 2.4 then imply that the domains of these resolvent functions are not only dense but actually all of $\mathcal{H}$. So every non-real complex number is in the resolvent set.

By Proposition 3.1 the approximate point spectrum is contained in $\mathbb{R}$ and by Proposition 3.4 there is no residual spectrum, so there is no part of σ_{ap} outside $\sigma_p \cup \sigma_c$. □

Suppose S and T are symmetric operators and $\overline{S} \subset S^{\dagger} \subset \overline{T} \subset T^{\dagger}$. Then

$$T^{\dagger\dagger} = \overline{T} \subset T^{\dagger} \subset S^{\dagger\dagger} = \overline{S} \subset S^{\dagger}.$$

In other words $\overline{T} = \overline{S} = S^{\dagger}$ and $\overline{S}$ is, therefore, self-adjoint.

We can draw conclusions from this.

First, there could be no self-adjoint extension of $S^{\dagger}$ for symmetric S other than, possibly, $S^{\dagger}$ itself.

More, $S^{\dagger}$ can not even have a nontrivial *symmetric* extension (that is, a symmetric extension bigger than itself) and if $S^{\dagger}$ is symmetric it must be self-adjoint.

Looking at this from the "T standpoint," if T is *any* symmetric operator, $\overline{T}$ cannot be a nontrivial extension of the adjoint of *any* symmetric operator.

So not only can there be no nontrivial "chains" of self-adjoint operators, there cannot even be nontrivial containment chains of *symmetric* operators, where the adjoint of one is contained in the closure of the next.

This implies, for instance, that different self-adjoint extensions of symmetric S, should there be more than one, cannot be compatible in the sense that neither could be an extension of the other.

On the other hand, suppose $S \subset \overline{T} \subset T^\dagger$. Then $T^{\dagger\dagger} = \overline{T} \subset T^\dagger \subset S^\dagger$ so

$$\overline{S} \subset \overline{T} \subset T^\dagger \subset S^\dagger.$$

We find that if S is a restriction of *any* symmetric operator, then S is symmetric too and any possible self-adjoint extension of S must lie between $\overline{S}$ and $S^\dagger$.

In the hunt for $\overline{T}$ for which $\overline{T} = T^\dagger$, increasing the size of $\mathcal{D}_{\overline{T}}$ decreases the size of $\mathcal{D}_{T^\dagger}$ *and there might be no way to "meet in the middle."* Some symmetric operators have no self-adjoint extension at all. Later, we examine a condition that will guarantee such extensions.

We say that unbounded T is **essentially self-adjoint** if $\overline{T} = T^\dagger$. By the discussion above this implies that $\overline{T}$ is the only self-adjoint extension of T. And there can there be no nontrivial self-adjoint restrictions of $\overline{T}$.

In the physics literature, the term **Hermitian operator** may refer to any of the operators we describe as symmetric, self-adjoint and essentially self-adjoint, depending on the predilections of the author. Busy physicists sometimes prefer not to think about the distinction unless absolutely necessary.

4. Counterexamples: Self-Adjointness

Here are a few very simple examples/counterexamples of the phenomena under consideration.

First we examine ***an operator that is not closeable*** and ***an adjoint without dense domain***.

Define T on $\mathcal{D}_T = C([0,1])$ by $T(\psi) = \psi(0)$, the constant function. So T is an unbounded operator on the Hilbert space $\mathcal{H} = \mathcal{L}^2([0,1])$.

Strictly speaking, of course, we are saying that members of $\mathcal{D}_T$ are those equivalence classes of measurable functions on $[0,1]$ that differ from a continuous function on a null set. There is at most one continuous function in any such class. T uses that member in its definition and returns the class of the relevant constant function.

$g \in \mathcal{D}_{T^\dagger}$ provided

$$\langle\, T(\psi)\,,\, g\,\rangle = \int_0^1 \overline{g(x)}\,\psi(0)\,dx = \psi(0)\int_0^1 \overline{g(x)}\,dx$$

is a bounded operator. But there is no limit to how large $\psi(0)$ can be among ψ of norm 1 in the Hilbert space, so we must have $\int_0^1 \overline{g(x)}\,dx = 0$. In other words, $\mathcal{D}_{T^\dagger} = 1^\perp$ which *is not* dense in $\mathcal{H}$.

And then for $g \in 1^\perp$ we have

$$\langle\, \psi\,,\, T^\dagger(g),\rangle = \langle\, T(\psi)\,,\, g\,\rangle = \psi(0)\int_0^1 \overline{g(x)}\,dx = 0.$$

So $T^\dagger$ is the zero operator on $1^\perp$.

Next, we look at an example of ***an operator that is symmetric but not essentially self-adjoint.***

Consider the operator $S = i\,\frac{d}{dx}$ defined on $\mathcal{D}_S$, which consists of those members $f \in C^1([0,1])$ with $f(0) = f(1) = 0$. So S is an unbounded operator on the Hilbert space $\mathcal{H} = \mathcal{L}^2([0,1])$. S is symmetric.

$$\langle\, S(g)\,,\, f\,\rangle = \langle\, g\,,\, S(f)\,\rangle \quad \forall f, g \in \mathcal{D}_S$$

as shown by the calculation

$$\int_0^1 (i\,g'(x))\,\overline{f(x)}\,dx = i\,g(x)\,\overline{f(x)}\Big|_0^1 - \int_0^1 i\,g(x)\,\overline{f'(x)}\,dx$$
$$= g(1)\overline{f(1)} - g(0)\overline{f(0)} \;+\; \int_0^1 g(x)\,\overline{(\,i\,f'(x)\,)}\,dx.$$

Let E_t consist of those members f of $C^1([0,1])$ for which $f(1) = e^{it}f(0)$ for a fixed real t. And let A_t be the operator with the same formula as S but defined on E_t. For these functions

$$g(1)\overline{f(1)} - g(0)\overline{f(0)} = e^{it}g(0)e^{-it}\overline{f(0)} - g(0)\overline{f(0)} = 0$$

so the A_t are symmetric by the same calculation used above for S and are extensions of S. Note that the A_t are incompatible except for values of t for which they are equal: they cannot have a shared self-adjoint extension.

So either symmetric S has multiple incompatible self-adjoint extensions or no more than one of the A_t has a self-adjoint extension at all.

The next example features ***a symmetric operator whose adjoint is not symmetric, and therefore (of course) not self-adjoint.***

The set $C = C_c^\infty(\,(0,1)\,)$ consists of those infinitely differentiable functions on $(0,1)$ which are 0 off some compact subinterval of $(0,1)$.

C may be considered as a dense subset of $\mathcal{L}^2([0,1])$.

We define operator T_C by the formula $-\frac{d^2}{dx^2}$ applied to members of C.

Suppose f and g are in C. Then since members of C and all their derivatives are 0 on the boundary of $[0,1]$

$$\langle\, T_C(f)\,,\, g\,\rangle = \int_0^1 -f''(x)\,g(x)\,dx = \int_0^1 f'(x)\,g'(x)\,dx$$
$$= \int_0^1 -f(x)\,g''(x)\,dx = \langle\, f\,,\, T_C(g)\,\rangle.$$

So T_C is symmetric.

For any $f \in C$ we have

$$\langle\, T_C(f)\,,\, 1\,\rangle = \int_0^1 -f''(x)\,dx = -f'(x)\Big|_0^1 = -f'(1) + f'(0) = 0.$$

So this functional is (very) bounded and $1 \in \mathcal{D}_{T_C^\dagger}$ and $T_C^\dagger(1) = 0$.

We have discovered that $(1,0) \in T_C^\dagger$.

Note that for any twice differentiable f and $x \in [0,1]$ we have

$$\left|\int_0^x \int_0^t f''(s)\,ds\,dt\right| = \left|\int_0^x f'(t) - f'(0)\,dt\right| = |f(x) - x\,f'(0) - f(0)|\,.$$

In case $f \in C$ we have then

$$| f(x) | = \left| \int_0^x \int_0^t f''(s)\, ds\, dt \right| \leq \int_0^x \int_0^t | f''(s) |\, ds\, dt \leq \int_0^1 \int_0^1 | f''(s) |\, ds\, dt$$
$$= \int_0^1 | f''(s) |\, ds \leq \sqrt{\int_0^1 | f''(s) |^2\, ds} = \| T_C(f) \|$$

where the last inequality is Jensen's inequality applied to the squaring function.

So if f_n is a sequence in C for which $\| T_C(f_n) \|$ converges to 0 then the sequence f_n *cannot* converge to 1, and that means $(1,0) \notin \overline{T_C}$.

The domain of the closed operator $T_C^\dagger$ is therefore strictly larger than the domain of $T_C^{\dagger\dagger} = \overline{T_C}$ so $T_C^\dagger$ is *not* symmetric.

And so $\overline{T_C}$, which is symmetric, is *not* self-adjoint.

5. When is an Operator Essentially Self-Adjoint?

We will now delve into means by which we can show a symmetric operator to be self-adjoint, or essentially self-adjoint.

We deal with the easiest case first.

5.1. ***Proposition***. ***Test for Essential Self-Adjointness.***
Suppose T is a symmetric operator and there is a real number α for which $\mathcal{R}_{\overline{T}-\alpha I} = \mathcal{H}$. Then $\overline{T}$ is self-adjoint.

Proof. Our goal below is to show that $\mathcal{D}_{T^\dagger} \subset \mathcal{D}_{\overline{T}}$ and, since the other containment is implied by the symmetry of $\overline{T}$, we will have $\overline{T} = T^\dagger$.

Assume the conditions on $\overline{T}$ and α. If $y \in \mathcal{D}_{T^\dagger}$ then since $\mathcal{R}_{\overline{T}-\alpha I} = \mathcal{H}$ we can find $w \in \mathcal{D}_{\overline{T}}$ for which $(\overline{T} - \alpha I)(w) = (T^\dagger - \alpha I)(y)$. Then $\forall x \in \mathcal{D}_{\overline{T}}$ we have

$$\langle (\overline{T} - \alpha I)(x) , y \rangle = \langle x , (T^\dagger - \alpha I)(y) \rangle$$
$$= \langle x , (\overline{T} - \alpha I)(w) \rangle = \langle (\overline{T} - \alpha I)(x) , w \rangle.$$

Since $\overline{T} - \alpha I$ is onto $\mathcal{H}$ this means $y = w$: that is, $y \in \mathcal{D}_{\overline{T}}$. □

The next few results rely only on **the symmetry condition** $\langle T(x) , y \rangle = \langle x , T(y) \rangle$ for members $x, y \in \mathcal{D}_T$ and not the density of $\mathcal{D}_T$ in $\mathcal{H}$, so we will assume T possesses the former property and not necessarily the latter.

If T has the symmetry condition it can have no complex eigenvalues. So if complex number α is not real the equation $T(g) = \alpha g$ has no solution except $g = 0$. This implies that $T - \alpha I$ is one-to-one from its domain $\mathcal{D}_T$ onto the set $\mathcal{R}_{T-\alpha I} = (T - \alpha I)(\mathcal{D}_T)$, where I is the identity operator on $\mathcal{H}$.

So the resolvent function $R_\alpha = (T - \alpha I)^{-1}$ is defined on the set $\mathcal{R}_{T-\alpha I}$.

A quick calculation shows that, since T has the symmetry condition, for any complex α

$$\langle (T - \alpha I)(x) , y \rangle = \langle x , (T - \overline{\alpha} I)(y) \rangle.$$

For T with the symmetry condition and non-real number α define C_α by

$$C_\alpha = (\,T - \overline{\alpha}\,I\,)(\,T - \alpha\,I\,)^{-1}$$

on the vector subspace $\mathcal{D}_{C_\alpha} = (\,T - \alpha\,I\,)(\mathcal{D}_T) = \mathcal{R}_{(T - \alpha\,I)}$ of $\mathcal{H}$.

The image of C_α is $\mathcal{R}_{C_\alpha} = C_\alpha\,(\mathcal{D}_{C_\alpha}) = (\,T - \overline{\alpha}\,I\,)(\mathcal{D}_T) = \mathcal{R}_{(T - \overline{\alpha}\,I)}$.

Note that $C_{\overline{\alpha}} \circ C_\alpha$ is the identity map on $\mathcal{D}_{C_\alpha}$.

It may be that $\mathcal{D}_{C_\alpha}$ fails to be dense in $\mathcal{H}$, which happens for symmetric T exactly when the number α is in the residual spectrum σ_r.

But dense domain or not, C_α is an isometry on its domain, as verified in the following calculation.

If $f = (\,T - \alpha\,I\,)(u)$ and $g = (\,T - \alpha\,I\,)(v)$ for $u, v \in \mathcal{D}_T$ expand and compare the right sides (using the symmetry condition) to show equality of the left sides.

$$\begin{aligned}\langle\, C_\alpha(f)\,,\, C_\alpha(g)\,\rangle &= \langle\,(\,T - \overline{\alpha}\,I\,)(u)\,,\,(\,T - \overline{\alpha}\,I\,)(v)\,\rangle\\ \langle\, f\,,\, g\,\rangle &= \langle\,(\,T - \alpha\,I\,)(u)\,,\,(\,T - \alpha\,I\,)(v)\,\rangle.\end{aligned}$$

The case of $\alpha = -i$ is singled out and called the **Cayley transform** of T with the symmetry condition. The Cayley transform

$$\mathbf{C(T)} = (\,T - i\,I\,)\,(\,T + i\,I\,)^{-1}$$

of T is an isometry from $(\,T + i\,I\,)(\mathcal{D}_T)$ onto $(\,T - i\,I\,)(\mathcal{D}_T)$.

Suppose $(\,T+i\,I\,)(x)$ is a generic member of the domain of $C(T)$. So this vector is also in the domain of $C(T) - I$, and

$$\begin{aligned}(\,C(T) - I\,)(\,T + i\,I\,)(x) &= C(T)(\,T + i\,I\,)(x) - (\,T + i\,I\,)(x)\\ &= (\,T - i\,I\,)(x) - (\,T + i\,I\,)(x) = -2\,i\,x.\end{aligned}$$

So the range of $C(T) - I$ is $\mathcal{D}_T$, and since $T - i\,I$ is one-to-one so is $C(T) - I$.

The Cayley transform of an operator as above is not just any isometry. ***It is an isometry that moves every domain member except the zero vector.***

The domain of $(C(T) - I)^{-1}$ is $\mathcal{D}_T$, and $(C(T) - I)^{-1}$ sends x to $\frac{i}{2}\,(\,T + i\,I\,)(x)$.

Now we calculate

$$\begin{aligned}(\,C(T) + I\,)(\,T + i\,I\,)(x) &= C(T)(\,T + i\,I\,)(x) + (\,T + i\,I\,)(x)\\ &= (\,T - i\,I\,)(x) + (\,T + i\,I\,)(x) = 2\,T(x).\end{aligned}$$

Putting these two calculations together yields

$$K(C(T))(x) = -i\,(\,C(T) + I\,)(C(T) - I)^{-1}(x) = T(x) \quad \forall x \in \mathcal{D}_T.$$

This operation K defined by

$$\mathbf{K(A)} = -i\,(\,A + I\,)(A - I)^{-1}$$

is called the **inverse Cayley transform**, and *it is defined for any isometry A which moves every domain member except 0*, required so that $A - I$ is one-to-one and $(A - I)^{-1}$ is defined.

Let's suppose $A\colon \mathcal{D}_A \to \mathcal{R}_A$ is any isometry of this type on $\mathcal{H}$.

Let $T = K(A)$. So $T\colon \mathcal{R}_{A-I} \to \mathcal{R}_{A+I}$.

If $x, y \in \mathcal{R}_{A-I}$ then $x = (A-I)(a)$ and $y = (A-I)(b)$ for certain $a, b \in \mathcal{D}_A$. But then

$$\begin{aligned}\langle\, T(x)\,,\, y\,\rangle &= \langle\, -i\,(A+I)(a)\,,\,(A-I)(b)\,\rangle \\ &= \,-\,i\;(\,\langle\, A(a)\,,\, A(b)\,\rangle - \langle\, A(a)\,,\, b\,\rangle + \langle\, a\,,\, A(b)\,\rangle - \langle\, a\,,\, b\,\rangle\,)\end{aligned}$$

and because A is an isometry this is $i\,(\langle\, A(a)\,,\, b\,\rangle - \langle\, a\,,\, A(b)\,\rangle\,)$. Similarly,

$$\begin{aligned}\langle\, x\,,\, T(y)\,\rangle &= \langle\;(A-I)(a)\,,\, -i\,(A+I)(b)\,\rangle \\ &= i\;(\,\langle\, A(a)\,,\, A(b)\,\rangle + \langle\, A(a)\,,\, b\,\rangle - \langle\, a\,,\, A(b)\,\rangle - \langle\, a\,,\, b\,\rangle\,)\end{aligned}$$

and this simplifies to the same number, so T has the symmetry condition.

If $T = K(A)$ is densely defined we now know that T is symmetric, though none of the calculations involving these transforms so far used this density. Dense domain or not, the symmetry condition implies that $T + i\,I$ and $T - i\,I$ are one-to-one on their common domain $\mathcal{D}_T = \mathcal{R}_{A-I}$.

Now suppose $x \in \mathcal{D}_A$ so $(A-I)(x)$ is a generic member of $\mathcal{D}_{K(A)}$.

$$\begin{aligned}\text{Then}\quad (\,K(A)\,+i\,I\,)(A-I)(x) &= K(A)(A-I)(x) + i\,(A-I)(x) \\ &= \,-\,i\,(A+I)(x) + i\,(A-I)(x) = -2i\,x.\end{aligned}$$

So $K(A) + i\,I$ is onto $\mathcal{D}_A$ and $x = \frac{i}{2}\,(\,K(A)\,+i\,I\,)(A-I)(x)$. Now we have

$$\begin{aligned}C(K(A))(x) &= (\,K(A)\,-i\,I\,)(\,K(A)\,+i\,I\,)^{-1}(x) \\ &= (\,K(A)\,-i\,I\,)(\,K(A)\,+i\,I\,)^{-1}\frac{i}{2}\,(\,K(A)\,+i\,I\,)(A-I)(x) \\ &= \frac{i}{2}\,(\,K(A)\,-i\,I\,)(A-I)(x) = \frac{i}{2}\,(\,-i\,(A+I)(x)\,-i\,(A-I)(x)\,) \\ &= A(x).\end{aligned}$$

Let's recapitulate.

1 is not an eigenvalue of any isometry produced by applying the Cayley transform to any operator that satisfies the symmetry condition; that is, the isometry thereby produced moves every member of its domain except 0. The inverse Cayley transform can be applied to any isometry from one subspace of $\mathcal{H}$ to another, so long as 1 is not an eigenvalue of this isometry. The operator produced satisfies the symmetry condition, and will be a symmetric operator if it has dense domain.

5.2. ***Proposition***. *If T has the with the symmetry condition then the Cayley transform $C(T)$ of T is an isometry with domain $\mathcal{D}_{C(T)} = (\,T + i\,I\,)(\mathcal{D}_T)$ onto range $\mathcal{R}_{C(T)} = (\,T - i\,I\,)(\mathcal{D}_T)$. This isometry moves every domain member except 0, and $K(C(T)) = T$.*

If A is any isometry extending $C(T)$ which moves every domain member except 0 then the inverse Cayley transform $K(A)$ of A is an extension of T with the symmetry condition and $C(K(A)) = A$.

Proof. Examine the remarks above. □

5.3. ***Lemma***. *Suppose T is symmetric.*

T is closed exactly when $\mathcal{R}_{T+i\,I}$ is closed.

T is closed exactly when $\mathcal{R}_{T-i\,I}$ is closed.

PROOF. For $x \in \mathcal{D}_T$ note that

$$\begin{aligned}&\langle\, (\, T + i\, I\,)(x)\, ,\, (\, T + i\, I\,)(x)\, \rangle \\ &\qquad = \langle\, T(x)\, ,\, T(x)\, \rangle + i\, \langle\, x\, ,\, T(x)\, \rangle - i\, \langle\, T(x)\, ,\, x\, \rangle + i(-i)\, \langle\, x\, ,\, x\, \rangle.\end{aligned}$$

By symmetry of T the middle terms cancel and we have, for every $x \in \mathcal{D}_T$,

$$\|\, (\, T + i\, I\,)(x)\, \|^2 = \|\, T(x)\, \|^2 + \|\, x\, \|^2.$$

Also by symmetry, $T + i\, I$ is one-to-one. So the map that sends $(\, T + i\, I\,)(x) \in \mathcal{R}_{T+i\, I}$ to $(x, T(x)) \in T$ is an isometry onto T with norm induced from $\mathcal{H} \times \mathcal{H}$. The two sets are closed or not together.

The situation with the operator $T - i\, I$ is identical. □

5.4. ***Lemma***. *If T is symmetric then $\overline{\mathcal{R}_{T-i\, I}} = \mathcal{R}_{\overline{T}-i\, I}$.*
Similarly, $\overline{\mathcal{R}_{T+i\, I}} = \mathcal{R}_{\overline{T}+i\, I}$.

PROOF. Expanding $\|\, (T - i\, I)(f)\, \|^2$ shows that $\|\, (T - i\, I)(f)\, \| \geq \|\, f\, \|\ \forall f \in \mathcal{D}_T$. That is, $T - i\, I$ is bounded below by 1. So if $(T - i\, I)(h_n) = T(h_n) - i\, h_n \in (T - i\, I)(\mathcal{D}_T)$ for $h_n \in \mathcal{D}_T$ is a Cauchy sequence then h_n must be Cauchy too and this implies $T(h_n)$ is Cauchy so $(h_n, T(h_n))$ converges to a point $(f, \overline{T}(f)) \in \overline{T}$. So $(T - i\, I)(h_n)$ converges to $(\overline{T} - i\, I)(f) \in (\overline{T} - i\, I)(\mathcal{D}_{\overline{T}})$, and we find that $\overline{(T - i\, I)(\mathcal{D}_T)} \subset (\overline{T} - i\, I)(\mathcal{D}_{\overline{T}})$.

The inclusion $(\overline{T} - i\, I)(\mathcal{D}_{\overline{T}}) \subset \overline{(T - i\, I)(\mathcal{D}_T)}$ is similar. □

5.5. ***Lemma***. *Symmetric T is self-adjoint exactly when*
its Cayley transform $C(T)$ is unitary.

PROOF. If T is self-adjoint then it is closed. By the last lemma so are $\mathcal{R}_{T+i\, I}$ and $\mathcal{R}_{T-i\, I}$. Also, $\mathcal{R}^{\perp}_{T+i\, I} = Ker(T^\dagger - i\, I) = Ker(T - i\, I) = \{\, 0\, \}$ since symmetric operators cannot have non-real eigenvalues. So $\mathcal{R}_{T+i\, I}$ is dense in $\mathcal{H}$ and so *is* $\mathcal{H}$. $\mathcal{R}_{T-i\, I}$ is found to be $\mathcal{H}$ by similar means. Since $C(T)$ is an isometry onto $\mathcal{H}$ it is unitary.

On the other hand suppose $C(T)$ is unitary. That means $\mathcal{R}_{T+i\, I} = \mathcal{R}_{T-i\, I} = \mathcal{H}$. Suppose that $x \in \mathcal{D}_T$ and $y \in \mathcal{D}_{T^\dagger}$ and select $w \in \mathcal{D}_T$ so that $(T - i\, I)(w) = (T^\dagger - i\, I)(y)$. Now we have

$$\begin{aligned}\langle\, (T + i\, I)(x)\, ,\, y\, \rangle &= \langle\, x\, ,\, (T^\dagger - i\, I)(y)\, \rangle = \langle\, x\, ,\, (T - i\, I)(w)\, \rangle \\ &= \langle\, (T^\dagger + i\, I)(x)\, ,\, w\, \rangle = \langle\, (T + i\, I)(x)\, ,\, w\, \rangle.\end{aligned}$$

Since $\mathcal{R}_{T+i\, I} = \mathcal{H}$ this means $y = w$, so $y \in \mathcal{D}_T$; so $\mathcal{D}_{T^\dagger} \subset \mathcal{D}_T$ and $T = T^\dagger$. □

We define the **deficiency subspaces** $\boldsymbol{\mathcal{D}_-}$ and $\boldsymbol{\mathcal{D}_+}$ by

$$\begin{aligned}\mathcal{D}_+ &= \,(\, \mathcal{R}_{T-i\, I}\,)^\perp = Ker\left(\, T^\dagger + i\, I\, \right) \\ &\text{and}\ \ \mathcal{D}_- = (\, \mathcal{R}_{T+i\, I}\,)^\perp = Ker\left(\, T^\dagger - i\, I\, \right).\end{aligned}$$

The **deficiency indices** $\boldsymbol{n_-}$ and $\boldsymbol{n_+}$ are the Hilbert dimensions of the respective deficiency subspaces.

If T is closed and symmetric then the following are orthogonal direct sums:

$$\mathcal{H} = \mathcal{R}_{T+i\,I} \oplus \mathcal{D}_- \quad \text{and} \quad \mathcal{H} = \mathcal{R}_{T-i\,I} \oplus \mathcal{D}_+.$$

The Cayley transform $C(T)\colon \mathcal{R}_{T+i\,I} \to \mathcal{R}_{T-i\,I}$ is an isometry onto $\mathcal{R}_{T-i\,I}$ which moves every nonzero member of its domain, so an isometry from $\mathcal{D}_-$ onto $\mathcal{D}_+$ which moves every nonzero member of $\mathcal{D}_-$, if there are any, could be combined with $C(T)$ to produce a unitary operator U on $\mathcal{H}$ extending $C(T)$. Then $K(U)$ is a self-adjoint extension of T.

5.6. ***Theorem***. *If T is symmetric then T has a self-adjoint extension if and only if the deficiency indices n_+ and n_- of T are equal. If $\mathcal{D}_+ = \mathcal{D}_- = \{\, 0 \,\}$ then $\overline{T}$ itself is self-adjoint. Otherwise, the distinct self-adjoint extensions of T correspond to those isometries from $\mathcal{D}_-$ onto $\mathcal{D}_+$ which leave no point of $\mathcal{D}_-$ except 0 unmoved. The association is through the inverse Cayley transform.*

Proof. The argument follows from the preceding discussions. □

5.7. ***Exercise***. *If $g \in \mathcal{D}_- \cap \mathcal{D}_+$ then $g \in (\mathcal{D}_T)^\perp \cap (\mathcal{R}_T)^\perp$. So if T is symmetric (i.e. it satisfies the symmetry condition and has dense domain) any isometry of $\mathcal{D}_-$ onto $\mathcal{D}_+$ whatsoever satisfies the condition in Theorem 5.6, since there are no shared points to leave unmoved except 0.*

Test for Essential Self-Adjointness *So symmetric T is essentially self-adjoint if and only if the deficiency indices are both 0. If the indices are both 1 there is a "circle" of extensions of T: if a and b are unit vectors and $\mathcal{D}_- = \mathbb{C}\,a$ and $\mathcal{D}_+ = \mathbb{C}\,b$ then the linear map sending a to $e^{i\,t}b$ is an isometry for each fixed real t. If the indices are equal but exceed 1 the group of isometries of $\mathcal{D}_-$ onto $\mathcal{D}_+$ is larger, and each one corresponds to a distinct self-adjoint extension of T.*

We now reprise some of the discussions specialized above for Cayley transforms to get (in some ways) a slightly more general result.

5.8. ***Theorem***. ***Test for Essential Self-Adjointness***
If T is symmetric and both $\mathcal{D}_{C_\alpha}$ and $\mathcal{D}_{C_{\overline{\alpha}}}$ are dense in $\mathcal{H}$ for some non-real complex number α then $\overline{T}$ is the unique self-adjoint extension of T.

Proof. Suppose first that symmetric T is closed and both domains are dense as indicated in the statement of this theorem.

Suppose also that $f_i = (\,T - \alpha\, I\,)(g_i) = T(g_i) - \alpha\, g_i$ is a Cauchy sequence in $\mathcal{D}_{C_\alpha}$ where g_i is a sequence in $\mathcal{D}_T$. Since C_α is an isometry, $C_\alpha(f_i) = (\,T - \overline{\alpha}\, I\,)(g_i) = T(g_i) - \overline{\alpha}\, g_i$ is also Cauchy. So the difference sequence

$$f_i - C_\alpha(f_i) = (T(g_i) - \alpha\, g_i) \;-\; (T(g_i) - \overline{\alpha}\, g_i) = (\overline{\alpha} - \alpha)\, g_i$$

is Cauchy and it follows that both g_i and $T(g_i)$ are Cauchy, and therefore converge to limits a and b, respectively, in $\mathcal{H}$.

Using the assumption that T is closed we conclude that $a \in \mathcal{D}_T$ and $b = T(a)$. Therefore $f_i = T(g_i) - \alpha\, g_i$ converges to $T(a) - \alpha\, a \in \mathcal{D}_{C_\alpha}$ and so $\mathcal{D}_{C_\alpha}$ is closed. Our assumption then that $\mathcal{D}_{C_\alpha}$ is dense implies that $\mathcal{D}_{C_\alpha} = \mathcal{H}$ and, similarly, $\mathcal{D}_{C_{\overline{\alpha}}} = \mathcal{H}$.

Now suppose that $f \in \mathcal{D}_{T^\dagger}$.

By definition of adjoint, $\left(T^\dagger - \alpha\, I\right)(f)$ is the unique member of $\mathcal{H}$ for which

$$\langle\, f\, ,\, (\, T - \overline{\alpha}\, I\,)\,(h)\,\rangle = \langle\, \left(T^\dagger - \alpha\, I\right)(f)\, ,\, h\,\rangle \qquad \forall h \in \mathcal{D}_T.$$

Because $(\, T - \alpha\, I\,)(\mathcal{D}_T) = \mathcal{D}_{C_\alpha} = \mathcal{H}$ there is a member g of $\mathcal{D}_T$ for which

$$(\, T - \alpha\, I\,)(g) = (\, T^\dagger - \alpha\, I\,)(f).$$

But then for every $h \in \mathcal{D}_T$

$$\begin{aligned}\langle\, f\, ,\, (\, T - \overline{\alpha}\, I\,)\,(h)\,\rangle &= \langle\, \left(T^\dagger - \alpha\, I\right)(f)\, ,\, h\,\rangle \\ &= \langle\, (\, T - \alpha\, I\,)\,(g)\, ,\, h\,\rangle = \langle\, g\, ,\, (\, T - \overline{\alpha}\, I\,)\,(h)\,\rangle\end{aligned}$$

where the last equality follows from symmetry of T.

Since $(\, T - \overline{\alpha}\, I\,)(\mathcal{D}_T) = \mathcal{D}_{C_{\overline{\alpha}}} = \mathcal{H}$ this means $f = g$. But $g \in \mathcal{D}_T$ by assumption. So $\mathcal{D}_{T^\dagger} \subset \mathcal{D}_T$. By the symmetry of T we know $\mathcal{D}_T \subset \mathcal{D}_{T^\dagger}$. So $T = T^\dagger$. Since T is closed $T^{\dagger\dagger} = T = T^\dagger$.

Now we remove the assumption that T is closed. Then $T \subset \overline{T} \subset T^\dagger$. The domain of $\overline{T}$ contains that of T so the domain of C_α calculated for $\overline{T}$ contains that of the similar transform found using T for each non-real α, so the density condition of this theorem for T implies the density condition for $\overline{T}$.

So $\overline{T} = T^\dagger$. Since $\overline{T}$ is the smallest possible extension of T which *could* be self-adjoint, and since there can be no proper self-adjoint extensions of a known self-adjoint extension, $\overline{T}$ is the unique self-adjoint extension of T. □

5.9. ***Exercise***. *(i)* ***Test for Essential Self-Adjointness.*** *Review Exercise 1.9 and prove that if T is symmetric and there is any non-real complex number α such that neither α nor $\overline{\alpha}$ is an eigenvalue of $T^\dagger$ then T is essentially self-adjoint and $\overline{T}$ is self-adjoint. (hint: $Ker(T^\dagger - \overline{\alpha}\, I) = (\,\mathcal{D}_{C_\alpha}\,)^\perp$.)*

(ii) If T is symmetric and there is a single non-real α for which neither α nor $\overline{\alpha}$ is an eigenvalue for $T^\dagger$ then no non-real β is an eigenvalue for $T^\dagger$.

(iii) If symmetric T fails to be essentially self-adjoint, at least one of β or $\overline{\beta}$ is an eigenvalue of $T^\dagger$ for every non-real β, and therefore at least one of β or $\overline{\beta}$ is in the residual spectrum of T.

(iv) ***Test for Essential Self-Adjointness.*** *Show that if T is symmetric, $\overline{T}$ is self-adjoint if and only if for every Cauchy sequence x_n of unit vectors in $\mathcal{D}_T$ for which $T(x_n)$ is also Cauchy, neither $(T + i\, I)(x_n)$ nor $(T - i\, I)(x_n)$ converges to 0.*

This is equivalent to the following: $\overline{T}$ is self-adjoint if and only if for any Cauchy sequence x_n of vectors in $\mathcal{D}_T$ for which $T(x_n)$ is also Cauchy, if either $(T + i\, I)(x_n) \to 0$ or $(T - i\, I)(x_n) \to 0$ then $x_n \to 0$.

(v) In Lemma 2.6 we determined that a (possibly small) disk around every member of the resolvent set is also in the resolvent set. If λ is real and in the resolvent set then there will be some non-real α for which both α and $\overline{\alpha}$ are in the resolvent set. So we have the following:

Test for Essential Self-Adjointness. *If T is symmetric, $\overline{T}$ is self-adjoint if there is a real number λ in the resolvent set.*

6. Examples: Self-Adjointness

Here is an example of ***incompatible essentially self-adjoint extensions of a symmetric operator.***

Let D consist of the infinitely differentiable functions f defined on $[0,1]$ (one-sided derivatives at the endpoints) with Dirichlet boundary conditions: $f(0) = f(1) = 0$. Let N consist of the infinitely differentiable functions f defined on $[0,1]$ with Neumann boundary conditions: $f'(0) = f'(1) = 0$.

Define operators T_D and T_N on D and N respectively by the same formula

$$T_D(f) = -f'' \quad \forall f \in D, \qquad T_N(f) = -f'' \quad \forall f \in N.$$

As in the example on page 21, both domains may be considered as a dense subset of $\mathcal{L}^2([0,1])$, and with that assumption both of these operators extend T_C, which was shown to be *not* essentially self-adjoint by explicitly producing a point on the graph of $T_C^\dagger$ which was not in $\overline{T_C}$.

$$\begin{aligned}\langle\, T_D(f)\,,\, g\,\rangle &= \int_0^1 -f''(x)\, g(x)\, dx = -f'(x)g(x)\Big|_0^1 + \int_0^1 f'(x)\, g'(x)\, dx \\ &= \; - f'(x)g(x)\Big|_0^1 + f(x)g'(x)\Big|_0^1 - \int_0^1 f(x)\, g''(x)\, dx = \; \langle\, f\,,\, T_D(g)\,\rangle.\end{aligned}$$

So T_D is symmetric, and the same calculation reveals T_N to be symmetric too.

Let's examine $(T_D + i\,I)(\mathcal{D}_{T_D})$. For integers n we find that $(T_D + i\,I)(\,\sin(n\pi x)\,) = (-n^2\pi^2 + i)\sin(n\pi x)$ and the finite linear combinations of functions of this type form a dense subset of D, and hence of $\mathcal{L}^2([0,1])$ itself. Also finite linear combinations of functions of the form $(T_D - i\,I)(\,\sin(n\pi x)\,) = (-n^2\pi^2 - i)\sin(n\pi x)$ are dense. Therefore $\overline{T_D}$ is self-adjoint.

Similar statements involving $(T_N + i\,I)(\,\cos(n\pi x)\,) = (-n^2\pi^2 + i)\cos(n\pi x)$ and $(T_N - i\,I)(\,\cos(n\pi x)\,) = (-n^2\pi^2 - i)\cos(n\pi x)$ allow us to conclude that T_N is also essentially self-adjoint.

Appealing to Exercise 5.9 and referring again to the example on page 21 we can also conclude that for every non-real α *at least one of* α *or* $\overline{\alpha}$ is an eigenvalue of $T_C^\dagger$ but *neither* α *nor* $\overline{\alpha}$ is an eigenvalue of either $T_N^\dagger$ or $T_D^\dagger$.

6.1. ***Lemma***. *If S is symmetric and $T \subset S$ and*
$(T + i\,I)(\mathcal{D}_T) = (S + i\,I)(\mathcal{D}_S)$ then $T = S$.

PROOF. Suppose $(S + i\,I)(f)$ for $f \in \mathcal{D}_S$ is some member of the range of $S + i\,I$. Since the ranges of $S + i\,I$ and $T + i\,I$ are equal, there must be a $g \in \mathcal{D}_T$ for which $(T + i\,I)(g) = (S + i\,I)(f)$. But S extends T so $(S + i\,I)(g) = (S + i\,I)(f)$. Since S is symmetric $S + i\,I$ is one-to-one so $f = g$. That means $\mathcal{D}_S \subset \mathcal{D}_T$. □

Finally, we look at an example of ***a symmetric operator with no self-adjoint extension at all.***

We will let our Hilbert space be $\boldsymbol{\ell^2}$, the space of square summable sequences with orthonormal basis e_n given by $e_n(j) = 1$ if $j = n$ and $e_n(j) = 0$ otherwise, for $n \geq 0$.

Define $s_n = e_n - e_{n+1}$ for $n \geq 0$. The set of these s_n is linearly independent, and if $f \in \boldsymbol{\ell^2}$ and $\langle f, s_n \rangle = 0$ for all n it is pretty easy to show that f is the zero sequence.

So the vector space formed from the finite linear combinations of these s_n, which we will denote $\mathcal{D}_T$, is dense in $\boldsymbol{\ell^2}$.

We define T on $\mathcal{D}_T$ by $T(s_n) = i\,e_n + i\,e_{n+1}$, extending by linearity.

A quick calculation verifies that $\langle T(s_n), s_m \rangle$ and $\langle s_n, T(s_m) \rangle$ are equal, and in fact both inner products are i if $m = n+1$ and $-i$ if $m = n-1$ and 0 otherwise.

So T is symmetric.

$(T + i\,I)(s_n) = 2\,i\,e_n$ so the range of $T + i\,I$ is dense. So (Lemma 5.4) we find that $(\overline{T} + i\,I)(\mathcal{D}_{\overline{T}}) = \boldsymbol{\ell^2}$.

However $(T - i\,I)(s_n) = 2\,i\,e_{n+1}$ which means that $e_1 \in (\,(T - i\,I)(\mathcal{D}_T)\,)^\perp$. i is in the residual spectrum $\sigma_r(T)$ of T.

So $e_1 \in \left(\,(\overline{T} - i\,I)(\mathcal{D}_T)\,\right)^\perp$, by Lemma 5.4. So $(\overline{T} - i\,I)(\mathcal{D}_T)$ is not dense in $\boldsymbol{\ell^2}$ so $\overline{T}$ is not self-adjoint. Also, Theorem 5.6 tells us that this operator has no self-adjoint extension.

If S is symmetric closed extension of T then the range of $S + i\,I$ would necessarily contain $(\overline{T} + i\,I)(\mathcal{D}_{\overline{T}}) = \boldsymbol{\ell^2}$, so $(S + i\,I)(\mathcal{D}_{\overline{T}}) = (\overline{T} + i\,I)(\mathcal{D}_{\overline{T}})$. By Lemma 6.1 we then have $S = T$: in other words, T cannot even have a nontrivial *symmetric* extension. That fact could also be deduced by appeal to Theorem 5.6.

We are now in a position to efficiently deal with a case that is very common, possibly even the most important case, in applications.

6.2. ***Theorem*. *Test for Essential Self-Adjointness.***
Suppose T has the symmetry condition and $\mathcal{H}$ has an orthonormal basis B of eigenvectors of T, with eigenvalue λ_b for each $b \in B$.
Then the domain of T is dense and $\overline{T}$ is self-adjoint and $\sigma\left(\overline{T}\right) = \overline{\{\,\lambda_b \mid b \in B\,\}}$.

Proof. $\mathcal{D}_T$ must contain the dense set *span*(B), the finite linear combinations of members of B, so T is symmetric and so too then is $\overline{T}$, defined on $\mathcal{D}_{\overline{T}}$. The orthonormal basis B is contained in $\mathcal{R}_{\overline{T}+i\,I}$ and $\mathcal{R}_{\overline{T}-i\,I}$, which are closed and dense and hence equal $\mathcal{H}$. By Theorem 5.8 $\overline{T}$ is self-adjoint, and we know that $\overline{T}$ must be contained in any possible self-adjoint extension of T so T is essentially self-adjoint.

Let L denote $\overline{\{\,\lambda_b \mid b \in B\,\}}$. The eigenvalues of T are all eigenvalues of $\overline{T}$ and the spectrum of any operator is closed, so $L \subset \sigma(\overline{T})$.

Suppose a is any number not in L. Suppose the distance from a to L is d. Given generic $x = \sum_{b \in B} a_b\, b$ define

$$F(x) = \sum_{b \in B} \frac{a_b}{\lambda_b - a}\, b.$$

The denominators in this formula are never smaller than d, so the operator norm of F does not exceed $1/d$. F is one-to-one and its range contains every member of B, so is dense in $\mathcal{H}$.

$$(T - a\,I) \circ F(b) = b = F \circ (T(b) - a\,b) \quad \forall b \in B.$$

So F is the resolvent $R_a(\overline{T})$, continuous and densely defined. So $a \notin \sigma\left(\overline{T}\right)$. □

We note here that the eigenvalues of this theorem could be dense in any subset (or all of) $\mathbb{R}$, so the spectrum could be any closed subset of $\mathbb{R}$.

7. The Friedrichs Extension

We now consider a condition for which a symmetric operator does have at least one self-adjoint extension.

We say operator T is **semi-bounded** (from below) if there is a real constant c for which

$$\langle T(g)\,,\,g\,\rangle \geq c\,\langle\,g\,,\,g\,\rangle \quad \forall g \in \mathcal{D}_T$$

and **positive** if c can be chosen to be 0 and **positive definite** if it is positive and $\langle T(g)\,,\,g\,\rangle = 0$ only when $g = 0$. If $c > 0$ we will call T **strongly positive**. We will refer to the greatest such c as **the lower semi-bound for T**.

$\langle T(g)\,,\,g\,\rangle$ is assumed to be real in this definition for all g, so semi-bounded operators are symmetric. That means the approximate point spectrum is a subset of the real numbers. But even more, the approximate point spectrum must be in $[c,\infty)$. To see this we select $\alpha \in \sigma_{ap}$. Then there is a sequence x_n of unit vectors in $\mathcal{D}_T$ with $\langle T(x_n)\,,\,x_n\,\rangle \to \alpha$. But by the semi-bound condition $\langle T(x_n)\,,\,x_n\,\rangle \geq c$ for each n and so $\alpha \in [c,\infty)$.

Note the distinction between semi-bounded and bounded below: T is bounded below if there is a *positive* c for which

$$\langle T(g)\,,\,T(g)\,\rangle \geq c\,\langle\,g\,,\,g\,\rangle \quad \forall g \in \mathcal{D}_T.$$

This latter condition is used for different purposes than the one we deal with now; for instance, T has bounded inverse exactly when it is bounded below.

In any event, if T is *semi-bounded* with constant c then $\langle T(g) - c\,g\,,\,g\,\rangle \geq 0$ and in fact if I is the identity operator,

$$\langle T(g) - c\,g + g\,,\,g\,\rangle = \langle\,(\,T - (c-1)\,I\,)(g)\,,\,g\,\rangle \geq \langle\,g\,,\,g\,\rangle \quad \forall g \in \mathcal{D}_T.$$

For this reason, many facts involving semi-bounded operators with any lower semi-bound are easy consequences of similar facts about positive operators, or semi-bounded operators with lower semi-bound 1.

In an attempt to find a self-adjoint extension for symmetric S we are looking for operator T with $\overline{S} \subset T = T^{\dagger} \subset S^{\dagger}$.

$\overline{S}$ is one possibility, and the domain of $\overline{S}$ can be described using a modified inner product, the graph inner product, on $\mathcal{D}_S$.

$$\langle\,g\,,\,h\,\rangle_G = \langle\,g\,,\,h\,\rangle + \langle\,S(g)\,,\,S(h)\,\rangle \quad \forall g,h \in \mathcal{D}_S.$$

Any Cauchy sequence in $\mathcal{D}_S$ using this inner product—we will call such sequences G-Cauchy—is also Cauchy with the Hilbert space inner product, and will converge in both senses to the same limit in $\mathcal{D}_{\overline{S}}$. Conversely, every member of $\mathcal{D}_{\overline{S}}$ is the limit of a G-Cauchy sequence. And the values of $\overline{S}$ on such a limit are the limits of the S-values on any G-Cauchy sequence in $\mathcal{D}_S$ converging to that limit vector.

Limits of G-Cauchy sequences not already in $\mathcal{D}_S$ are exactly the members of $\mathcal{D}_{\overline{S}}$ not already in $\mathcal{D}_S$. In other words, $\mathcal{D}_{\overline{S}}$ is the G-completion of $\mathcal{D}_S$.

In many cases $\overline{S}$ is not self-adjoint, and a self-adjoint extension of S, if one exists, will have larger domain. Our goal below is to find such an extension in a special case commonly found in applications.

Suppose now that S is not just symmetric but also semi-bounded with constant 1. Any operator with positive lower semi-bound must be one-to-one, and that is the case here.

First, we define the Friedrichs inner product and norm on $\mathcal{D}_S$ as follows.

$$\langle\, g\,,\, h\,\rangle_F = \langle\, S(g)\,,\, h\,\rangle \quad \text{and} \quad \|\, g\,\|_F = \sqrt{\langle\, g\,,\, g\,\rangle_F} \qquad \forall g, h \in \mathcal{D}_S.$$

Both the positive lower semi-bound constant and symmetry are needed to show that this is, indeed, an inner product on $\mathcal{D}_S$.

Now suppose a sequence g_n is in $\mathcal{D}_S$. Using the lower semi-bound constant and the BCS inequality,

$$\begin{aligned}\|\, g_n - g_m\,\|^2 \leq \|\, g_n - g_m\,\|_F^2 &= \langle\, S(g_n - g_m)\,,\, g_n - g_m\,\rangle \\ &\leq \|\, S(g_n - g_m)\,\|\,\|\, g_n - g_m\,\|.\end{aligned}$$

If the sequence g_n is G-Cauchy, both g_n and $S(g_n)$ are Cauchy. So the right side of this inequality can be made small by choosing m and n large enough. Then $\|\, g_n - g_m\,\|_F$ can also be made small by choosing m and n large enough. In other words, a G-Cauchy sequence is also F-Cauchy.

Looking at the left side of the inequality, we see that every F-Cauchy sequence is Cauchy in $\mathcal{H}$, and therefore converges in both senses to the same member of $\mathcal{H}$.

So if $\mathcal{K}$ is the F-completion of $\mathcal{D}_S$ we have

$$\mathcal{D}_S \subset \mathcal{D}_{\overline{S}} \subset \mathcal{K} \subset \overline{\mathcal{D}_S} = \mathcal{H}.$$

We extend the Friedrichs inner product to all of $\mathcal{K}$ by continuity. In particular, we note that since $\langle\, g\,,\, g\,\rangle_F = \langle\, S(g)\,,\, g\,\rangle \geq \langle\, g\,,\, g\,\rangle$ for all $g \in \mathcal{D}_S$ we also have $\langle\, g\,,\, g\,\rangle_F \geq \langle\, g\,,\, g\,\rangle$ for all $g \in \mathcal{K}$.

Then $\mathcal{K}$ is itself a Hilbert space with Fredrichs inner product, and by definition $\mathcal{D}_S$ is F-dense in $\mathcal{K}$.

For each $y \in \mathcal{H}$ the linear function

$$A_y(\cdot) = \langle\, \cdot\,,\, y\,\rangle \colon \mathcal{D}_S \to \mathbb{C}$$

has F-operator norm bound $\|\, y\,\|$, as calculated below:

$$|\, A_y(x)\,| = |\,\langle\, x\,,\, y\,\rangle\,| \leq \|\, x\,\|\,\|\, y\,\| \leq \|\, x\,\|_F\,\|\, y\,\|.$$

Since $\mathcal{D}_S$ is F-dense in $\mathcal{K}$, A_y corresponds to F-inner product against a unique member $w_y \in \mathcal{K}$: $A_y(\cdot) = \langle\, \cdot\,,\, w_y\,\rangle_F$, and w_y has F-norm not exceeding $\|\, y\,\|$.

We define $B(y) = w_y$ for every $y \in \mathcal{H}$. Then $B\colon \mathcal{H} \to \mathcal{K}$ is easily seen to be linear; $B(y)$ is the unique member of $\mathcal{K}$ for which

$$\langle\, x\,,\, B(y)\,\rangle_F = \langle\, x\,,\, y\,\rangle \quad \forall x \in \mathcal{D}_S.$$

We will now accumulate some properties of B.

If $x \in \mathcal{K}$ and $y \in \mathcal{H}$ and $B(y) = 0$ then

$$\langle\, x \,,\, 0 \,\rangle = \langle\, x \,,\, 0 \,\rangle_F = \langle\, x \,,\, B(y) \,\rangle_F = \langle\, x \,,\, y \,\rangle$$

and the density of $\mathcal{K}$ in $\mathcal{H}$ implies $y = 0$. So B is one-to-one.

B is symmetric with respect to the original inner product, as seen below. For any $x, y \in \mathcal{H}$ we have

$$\langle\, B(x) \,,\, y \,\rangle = \langle\, B(x) \,,\, B(y) \,\rangle_F = \overline{\langle\, B(y) \,,\, B(x) \,\rangle_F} = \overline{\langle\, B(y) \,,\, x \,\rangle} = \langle\, x \,,\, B(y) \,\rangle.$$

So B is self-adjoint and, by the Hellinger-Toeplitz theorem, continuous.

Also B is positive because $\forall x \in \mathcal{H}$

$$\langle\, B(x) \,,\, x \,\rangle = \langle\, B(x) \,,\, B(x) \,\rangle_F \geq \langle\, B(x) \,,\, B(x) \,\rangle \geq 0.$$

Since $B = B^\dagger$ and $(\mathcal{R}_B)^\perp = Ker\left(B^\dagger\right) = Ker\,(B) = \{\, 0 \,\}$ we know that the subset $\mathcal{R}_B$ of $\mathcal{K}$ is dense in $\mathcal{H}$. So B^{-1}, which we will henceforth denote by Q, is a symmetric operator $Q \colon \mathcal{R}_B \to \mathcal{H}$ and is onto $\mathcal{H}$.

Note that if $x, y \in \mathcal{D}_S$ then

$$\langle\, x \,,\, y \,\rangle_F = \langle\, S(x) \,,\, y \,\rangle = \langle\, x \,,\, S(y) \,\rangle = \langle\, x \,,\, B \circ S(y) \,\rangle_F.$$

But then for each $y \in \mathcal{D}_S$, $\langle\, x \,,\, y - B \circ S(y) \,\rangle_F = 0 \ \forall x \in \mathcal{D}_S$.

Since $\mathcal{D}_S$ is F-dense in $\mathcal{K}$ we have $y = B \circ S(y) \ \forall y \in \mathcal{D}_S$.

There are a couple of interesting conclusions to be drawn from this. First, all of $\mathcal{D}_S$ is in $\mathcal{R}_B = \mathcal{D}_Q$. And, second, $Q(y) = S(y) \ \forall y \in \mathcal{D}_S$.

We now know that Q is a symmetric extension of S, and since B is a closed operator, so too is its inverse Q.

Suppose $x = B(y)$ is a generic member of the domain of Q.

$$\begin{aligned} \langle\, Q(x) \,,\, x \,\rangle &= \langle\, x \,,\, Q(x) \,\rangle = \langle\, B(y) \,,\, y \,\rangle = \langle\, B(y) \,,\, B(y) \,\rangle_F \\ &\geq \langle\, B(y) \,,\, B(y) \,\rangle = \langle\, x \,,\, x \,\rangle. \end{aligned}$$

So Q is semi-bounded with constant 1, the same lower semi-bound as S.

Let $\psi \colon \mathcal{H} \times \mathcal{H} \to \mathcal{H} \times \mathcal{H}$ be the map that switches coordinates, $\psi(x, y) = (y, x)$. So ψ sends any one-to-one operator to its inverse, and in particular $\psi(B) = Q$ and $\psi(Q) = B$.

Recall the notation and result of Lemma 1.6 and observe that $J \circ \psi = -\psi \circ J$.

As subsets of $\mathcal{H} \times \mathcal{H}$ we have (since $B = B^\dagger$ and Q is closed)

$$\begin{aligned} Q = &\ -Q = -\psi(B) = -\psi(\,(\,J(\,B^\dagger\,)\,)^\perp\,) = -\psi(\,(\,J(\,B\,)\,)^\perp\,) \\ &= (\,J(\,Q\,)\,)^\perp = Q^\dagger. \end{aligned}$$

So Q is self-adjoint.

7.1. ***Theorem***. *A symmetric and semi-bounded operator has a self-adjoint extension that is also semi-bounded with the same lower semi-bound constant.*

PROOF. Suppose T is symmetric and semibounded with lower semi-bound constant c. Then $S = T - (c-1)\,I$ is *also* symmetric with lower semi-bound 1. According to the remarks before the theorem, there is a self-adjoint extension Q of S with lower semi-bound constant 1. And then $Q+(c-1)\,I$ is a self-adjoint extension of T with lower semi-bound constant c. $\square$

The semi-bounded self-adjoint operator of this theorem is called the **Friedrichs extension of T**.

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