

UNBOUNDED OPERATORS ON HILBERT SPACES

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ABSTRACT. These are notes from the lecture course “Unbounded operators on Hilbert spaces” delivered at the School on Geometry and Physics in Białowieża from June 28 through July 2, 2021.

1. BASIC OPERATOR THEORY

1.1. Fundamentals.

Throughout these notes \mathcal{H} will denote a Hilbert space and $B(\mathcal{H})$ the space of all bounded operators on \mathcal{H} , i.e. linear maps $a: \mathcal{H} \rightarrow \mathcal{H}$ such that

$$\|a\| = \sup_{\|\xi\|=1} \|a\xi\| < +\infty \quad (1)$$

(the left-hand side of (1) is called the *norm* of a).

The set $B(\mathcal{H})$ is a unital $*$ -algebra under natural which means that not only is $B(\mathcal{H})$ a complex vector space with usual addition and scalar multiplication of linear operators, but additionally the composition of operators defines an associative and bi-linear multiplication of bounded operators and the identity operator $\mathbb{1}$ is the unit of this multiplication. Finally the operation of passing from $a \in B(\mathcal{H})$ to its *hermitian adjoint* (*adjoint* for short) defined by

$$\langle \varphi | a\psi \rangle = \langle a^* \varphi | \psi \rangle, \quad \varphi, \psi \in \mathcal{H}$$

is an anti-linear and anti-multiplicative involution on $B(\mathcal{H})$.

Fact. $B(\mathcal{H})$ is a Banach $*$ -algebra, i.e.

- $B(\mathcal{H})$ is a Banach space with the norm defined by (1),
- for any $a, b \in B(\mathcal{H})$ we have $\|ab\| \leq \|a\| \|b\|$,
- for any $a \in B(\mathcal{H})$ we have $\|a^*\| = \|a\|$.

Moreover for any $a \in B(\mathcal{H})$ the identity $\|a^*a\| = \|a\|^2$ holds, which means that $B(\mathcal{H})$ is a *C*-algebra*.

Example. Let $\mathcal{H} = \ell_2$, i.e. \mathcal{H} is the space of sequences $\psi = (\psi_n)_{n \in \mathbb{N}}$ of complex numbers such that $\sum_{n=1}^{\infty} |\psi_n|^2 < +\infty$. Let $s: \mathcal{H} \rightarrow \mathcal{H}$ be defined by

$$(s\psi)_n = \begin{cases} 0 & n = 1 \\ \psi_{n-1} & n > 1 \end{cases}, \quad \psi \in \ell_2.$$

Then $s \in B(\mathcal{H})$ (in fact $\|s\| = 1$) and

$$(s^*\psi)_n = \psi_{n+1}, \quad \psi \in \mathcal{H}, n \in \mathbb{N}.$$

Note that $s^*s = \mathbb{1}$, but $ss^* \neq \mathbb{1}$.

1.2. The spectrum.

Terminology 1. Let $a \in B(\mathcal{H})$.

- We say that a is *invertible* if there exists $b \in B(\mathcal{H})$ such that $ab = ba = \mathbb{1}$ (we write $b = a^{-1}$), it is worth noting that if a is such that there exist b, c satisfying $ab = \mathbb{1} = ca$, then $b = c$ and consequently a is invertible,
- the *spectrum* of a is

$$\sigma(a) = \{\lambda \in \mathbb{C} \mid \lambda \mathbb{1} - a \text{ is not invertible}\},$$

- the *resolvent set* of a is $\rho(a) = \mathbb{C} \setminus \sigma(a)$,
- the *resolvent* of a is the function

$$\rho(a) \ni \mu \mapsto (\mu \mathbb{1} - a)^{-1} \in B(\mathcal{H}),$$

- the *spectral radius* of a is $\text{sr}(a) = \sup\{|\lambda| \mid \lambda \in \sigma(a)\}$.

Theorem. Let $a \in B(\mathcal{H})$. Then

- (1) $\text{sr}(a) \leq \|a\|$,
- (2) $\sigma(a)$ is a non-empty compact subset of \mathbb{C} ,
- (3) the resolvent is a continuous (in fact holomorphic) function $\rho(a) \rightarrow B(\mathcal{H})$,
- (4) the limit $\lim_{m \rightarrow \infty} \|a^m\|^{\frac{1}{m}}$ exists and is equal to $\text{sr}(a)$.

Example. Let $\mathcal{H} = \mathbb{C}^2$ and $a = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$. Then $\sigma(a) = \{0\}$, so that $\text{sr}(a) = 0$, while $\|a\| = 1$. Note that $\|a^m\|^{\frac{1}{m}} = 1$ for $m = 1$ and 0 otherwise.

Example. Let $\mathcal{H} = L_2(\mathbb{R})$ and let $\mathcal{F} : \mathcal{H} \rightarrow \mathcal{H}$ be the Fourier transformation:

$$(\mathcal{F}\psi)(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ipx} f(x) dx, \quad \psi \in L_1(\mathbb{R}) \cap L_2(\mathbb{R}), p \in \mathbb{R}.$$

Now consider the functions:

$$\begin{aligned} \psi_0(x) &= \pi^{-\frac{1}{4}} e^{-\frac{x^2}{2}} \\ \psi_1(x) &= \sqrt{2} \pi^{-\frac{1}{4}} x e^{-\frac{x^2}{2}} \\ \psi_2(x) &= (\sqrt{2} \pi^{\frac{1}{4}})^{-1} (2x^2 - 1) e^{-\frac{x^2}{2}} \\ \psi_3(x) &= (\sqrt{3} \pi^{\frac{1}{4}})^{-1} (2x^3 - 3x) e^{-\frac{x^2}{2}} \end{aligned} \quad x \in \mathbb{R}.$$

Then

$$\mathcal{F}\psi_0 = \psi_0, \quad \mathcal{F}\psi_1 = i\psi_1, \quad \mathcal{F}\psi_2 = -\psi_2 \quad \text{and} \quad \mathcal{F}\psi_3 = -i\psi_3,$$

so $\{1, i, -1, -i\} \subset \sigma(\mathcal{F})$. In fact $\sigma(\mathcal{F}) = \{1, i, -1, -i\}$.

1.3. Certain classes of operators.

Terminology 2. Let $a \in B(\mathcal{H})$. The following table contains definitions of seven important classes of operators:

type of operator	characterization		
	algebraic	geometric	spectral
<i>normal</i>	$a^*a = aa^*$	$\forall \xi \in \mathcal{H} \ \ a\xi\ = \ a^*\xi\ $	
<i>self-adjoint</i>	$a = a^*$	$\forall \xi \in \mathcal{H} \ \langle \xi a\xi \rangle \in \mathbb{R}$	a is normal and $\sigma(a) \subset \mathbb{R}$
<i>positive</i>	$\exists b \ a = b^*b$	$\forall \xi \in \mathcal{H} \ \langle \xi a\xi \rangle \geq 0$	a is normal and $\sigma(a) \subset \mathbb{R}_+$
<i>projection</i>	$a^*a = a$	$\exists \mathcal{M} \ a\xi = \begin{cases} \xi & \xi \in \mathcal{M} \\ 0 & \xi \in \mathcal{M}^\perp \end{cases}$	a is normal and $\sigma(a) \subset \{0, 1\}$
<i>partial isometry</i>	$aa^*a = a$	$\exists \mathcal{M} \ \ a\xi\ = \begin{cases} \ \xi\ & \xi \in \mathcal{M} \\ 0 & \xi \in \mathcal{M}^\perp \end{cases}$	
<i>isometry</i>	$a^*a = \mathbb{1}$	$\forall \xi \in \mathcal{H} \ \ a\xi\ = \ \xi\ $	
<i>unitary</i>	$a^*a = aa^* = \mathbb{1}$	surjective isometry	a is normal and $\sigma(a) \subset \mathbb{T}$

In the third and fourth row of the table \mathcal{M} stands for a closed vector subspace.

Remark. It is worth mentioning that the condition $aa^*a = a$ defining a partial isometry is equivalent to $(a^*a)^2 = a^*a$, i.e. to a^*a being a projection.

Proposition. Let $a \in B(\mathcal{H})$ be normal. Then $\text{sr}(a) = \|a\|$.

Proof. For $n \in \mathbb{Z}_+$ define $b_n = a^{2^n}$. Then each b_n is normal and we have $b_n = b_{n-1}^2$. Thus

$$\begin{aligned} \|b_n\|^2 &= \|b_n^* b_n\| = \|(b_{n-1}^2)^* (b_{n-1}^2)\| = \|b_{n-1}^* b_{n-1}^* b_{n-1} b_{n-1}\| \\ &= \|b_{n-1}^* b_{n-1} b_{n-1}^* b_{n-1}\| \\ &= \|b_{n-1}^* b_{n-1}\|^2 = \|b_{n-1}\|^4, \end{aligned}$$

so that

$$\|b_n\|^{\frac{1}{2^n}} = (\|b_n\|^2)^{\frac{1}{2^{n+1}}} = (\|b_{n-1}\|^4)^{\frac{1}{2^{n+1}}} = \|b_{n-1}\|^{\frac{1}{2^{n-1}}}, \quad n \in \mathbb{N}.$$

It follows that the sequence $(\|a^m\|^{\frac{1}{m}})_{m \in \mathbb{N}}$ has a constant subsequence with value $\|b_0\| = \|a\|$. \square

Proposition. Let $a \in B(\mathcal{H})$ be self-adjoint. Then $\sigma(a) \subset \mathbb{R}$.

Proof. Take $\lambda \in \sigma(a)$ and decompose it as $\lambda = \alpha + i\beta$ with $\alpha, \beta \in \mathbb{R}$. Now for $n \in \mathbb{N}$ put $a_n = a - (\alpha - in\beta)\mathbf{1}$. It is easy to show that $\sigma(a_n) = \sigma(a) - (\alpha - in\beta)$, so $i(n+1)\beta = \lambda - (\alpha - in\beta) \in \sigma(a_n)$. In particular we must have

$$|i(n+1)\beta| \leq \|a_n\|, \quad n \in \mathbb{N}.$$

In other words for any $n \in \mathbb{N}$

$$(n^2 + 2n + 1)\beta^2 \leq \|a_n^* a_n\| = \|(a - \alpha\mathbf{1})^2 + n^2\beta^2\mathbf{1}\| \leq \|(a - \alpha\mathbf{1})^2\| + n^2\beta^2$$

which is only possible when $\beta = 0$. \square

1.4. Functional calculus.

Proposition. Let $a \in B(\mathcal{H})$ and $P \in \mathbb{C}[\cdot]$. Then

$$\sigma(P(a)) = \{P(\lambda) \mid \lambda \in \sigma(a)\}.$$

Proof. The statement is obvious if $\deg P \leq 0$. Assume that $\deg P \geq 1$ and we have

$$P(x) = \alpha_0 + \alpha_1 x + \cdots + \alpha_n x^n.$$

Take $\lambda \in \sigma(a)$. Then

$$\begin{aligned} \underbrace{P(\lambda)\mathbf{1} - P(a)}_A &= \sum_{k=0}^n \alpha_k \lambda^k - \sum_{k=0}^n \alpha_k a^k = \sum_{k=0}^n \alpha_k (\lambda^k - a^k) \\ &= \sum_{k=0}^n \alpha_k (\lambda\mathbf{1} - a) \left(\sum_{j=0}^{n-1} \lambda^j a^{n-j-1} \right) \\ &= \underbrace{(\lambda\mathbf{1} - a)}_B \underbrace{\sum_{k=0}^n \alpha_k \left(\sum_{j=0}^{n-1} \lambda^j a^{n-j-1} \right)}_C. \end{aligned}$$

Note that $BC = CB$, so if A were invertible then we would have $\mathbf{1} = B(CA^{-1})$ and $\mathbf{1}\mathcal{H} = (A^{-1}C)B$ and consequently B would be invertible. But $\lambda \in \sigma(a)$, so $P(\lambda)$ must belong to $\sigma(P(a))$. This shows that $P(\sigma(a)) \subset \sigma(P(a))$.

Now take $\mu \in \mathbb{C} \setminus P(\sigma(a))$ and let $\lambda_1, \dots, \lambda_m$ be the different zeros of the polynomial $Q(x) = \mu - P(x)$. Thus there exists $\gamma \in \mathbb{C} \setminus \{0\}$ and multiplicities k_1, \dots, k_m such that

$$\mu - P(x) = \gamma(\lambda_1 - x)^{k_1} \cdots (\lambda_m - x)^{k_m}.$$

Clearly $\lambda_1, \dots, \lambda_m$ do not belong to $\sigma(a)$ and consequently

$$\mu\mathbf{1} - P(a) = Q(a) = \gamma(\lambda_1\mathbf{1} - a)^{k_1} \cdots (\lambda_m\mathbf{1} - a)^{k_m}$$

is invertible as a product of invertible operators. Thus $\mu \in \rho(P(a))$ which proves that $P(\rho(a)) \subset \rho(P(a))$, i.e. $P(\sigma(a)) \supset \sigma(P(a))$. \square

Theorem. Let $a \in B(\mathcal{H})$ be self-adjoint. Then there exists a unique linear map $C(\sigma(a)) \rightarrow B(\mathcal{H})$ denoted by $f \mapsto f(a)$ such that

- if f is a polynomial function $f(x) = \sum_{k=0}^n \alpha_k x^k$ then $f(a) = \sum_{k=0}^n \alpha_k a^k$,
- $\|f(a)\| = \sup_{\lambda \in \sigma(a)} |f(\lambda)|$ for all $f \in C(\sigma(a))$.

Moreover

- for all $f, g \in C(\sigma(a))$ we have $(fg)(a) = f(a)g(a)$,
- for all $f \in C(\sigma(a))$ we have $f(a)^* = \overline{f(a)}$.

Definition. Let $a \in B(\mathcal{H})$ be self-adjoint. The mapping

$$C(\sigma(a)) \ni f \longmapsto f(a) \in B(\mathcal{H})$$

described above is called the *continuous functional calculus* for a .

Sketch of proof. First we note that for any $P \in \mathbb{C}[\cdot]$ the operator $P(a)$ is normal, so

$$\begin{aligned} \|P(a)\| &= \text{sr}(P(a)) = \sup\{|\mu| \mid \mu \in \sigma(P(a))\} \\ &= \sup\{|P(\lambda)| \mid \lambda \in \sigma(a)\} = \|\Psi(P)\|_\infty, \end{aligned}$$

where $\Psi: \mathbb{C}[\cdot] \rightarrow C(\sigma(a))$ is the restriction map.

It follows that there exists a unique linear map Φ defined on the range of Ψ into $B(\mathcal{H})$ such that

$$\begin{array}{ccc} \mathbb{C}[\cdot] & \xrightarrow{\psi} & \text{ran } \Psi \\ \downarrow P \mapsto P(a) & & \swarrow \Phi \\ B(\mathcal{H}) & & \end{array}$$

Moreover Φ is isometric.

Next, using the density of polynomial functions in $C(\sigma(a))$, we extend Φ uniquely to an isometry $C(\sigma(a)) \rightarrow B(\mathcal{H})$ which we denote by $f \mapsto f(a)$. Clearly if f is a Polynomial function, i.e. $f = \Psi(P)$ for some $P \in \mathbb{C}[\cdot]$ then $f(a)$ coincides with $P(a)$.

We check that

$$(fg)(a) = f(a)g(a) \quad \text{and} \quad f(a)^* = \overline{f(a)}$$

for polynomial functions (we use $a = a^*$ for the second property) and note that these remain true for all $f, g \in C(\sigma(a))$ via uniform approximation.

The uniqueness of the mapping $f \mapsto f(a)$ with the properties described in the theorem is clear. \square

We have the following alternative formulation of the previous theorem:

Theorem. Let $a \in B(\mathcal{H})$ be self-adjoint. Then there exists a unique unital $*$ -homomorphism $C(\sigma(a)) \rightarrow B(\mathcal{H})$ mapping the identity function

$$\sigma(a) \ni \lambda \longmapsto \lambda \in \mathbb{R}$$

to a . Moreover this map is isometric.

Theorem. Let $a \in B(\mathcal{H})$ be self-adjoint. Then for any $g \in C(\sigma(a))$ we have $\sigma(g(a)) = g(\sigma(a))$.

The above statement is known as the *spectral mapping theorem*.

Remark. if $a = a^*$ and $g \in C(\sigma(a), \mathbb{R})$ then $g(a)^* = \overline{g(a)} = g(a)$, i.e. $g(a)$ is self-adjoint.

Remark. A fully analogous statements about functional calculus and the spectral mapping theorem remain true after replacing the assumption that a is self-adjoint by the requirement that it is normal.

The uniqueness of the continuous functional calculus provides an easy proof of the following corollary:

Corollary. Let $a \in B(\mathcal{H})$ be self-adjoint and let $g \in C(\sigma(a), \mathbb{R})$. Then for any $f \in C(\sigma(g(a)))$ we have $f(g(a)) = (f \circ g)(a)$.

In the next theorem we extend the continuous functional calculus for a self-adjoint $a \in B(\mathcal{H})$ to all bounded Borel functions on the spectrum. The unital $*$ -algebra of all these functions will be denoted by $\mathcal{B}(\sigma(a))$.

Theorem. *Let $a \in B(\mathcal{H})$ be self-adjoint. Then there exists a unique unital $*$ -homomorphism $\mathcal{B}(\sigma(a)) \rightarrow B(\mathcal{H})$ denoted by $f \mapsto f(a)$ such that*

- if f is the identity function then $f(a) = a$,
- if $(f_n)_{n \in \mathbb{N}}$ is a uniformly bounded sequence of elements of $\mathcal{B}(\sigma(a))$ converging pointwise to f then for any $\xi \in \mathcal{H}$ we have $f_n(a)\xi \xrightarrow[n \rightarrow \infty]{} f(a)\xi$.

Moreover the mapping $\mathcal{B}(\sigma(a)) \ni f \mapsto f(a) \in B(\mathcal{H})$ extends the continuous functional calculus.

The homomorphism $f \mapsto f(a)$ described in the above theorem is called the *Borel functional calculus* for a .

Remark. As with the continuous functional calculus the Borel functional calculus can be extended in the analogous form to normal operators in place of self-adjoint ones.

Example. Let $a \in B(\mathcal{H})$ be self-adjoint and let $f: \sigma(a) \rightarrow \mathbb{C}$ be defined as

$$f(\lambda) = \begin{cases} 1 & \lambda \neq 0 \\ 0 & \lambda = 0 \end{cases}.$$

Then $f \in \mathcal{B}(\sigma(a))$ and $f(a)$ is the projection onto $\overline{\text{ran } a}$.

Indeed, let $p = f(a)$. Then p is a projection and $pa = a$, so for any $\xi \in \text{ran } a$, i.e. $\xi = a\eta$ for some η , we have

$$p\xi = pa\eta = a\eta = \xi.$$

Thus $\text{ran } a \subset \text{ran } p$ and consequently $\overline{\text{ran } a} \subset \text{ran } p$. Conversely, since f can be written as a pointwise limit of polynomial functions $(P_n)_{n \in \mathbb{N}}$ without constant term, if $\psi \in \ker a$ then

$$p\psi = \lim_{n \rightarrow \infty} P_n(a)\psi = 0$$

and it follows that $\ker p \supset \ker a$, so that $\text{ran } p \subset (\ker a)^\perp = \overline{\text{ran } a}$.

Definition. Let $a \in B(\mathcal{H})$ be self-adjoint. The projection onto $\overline{\text{ran } a}$ is called the *support* of a . It is denoted by $\mathfrak{s}(a)$.

1.5. Polar decomposition.

Theorem (Polar decomposition). *Let $a \in B(\mathcal{H})$. Then there exists a unique $(v, d) \in B(\mathcal{H}) \times B(\mathcal{H})$ such that*

- $a = vd$,
- d is positive,
- $v^*v = \mathfrak{s}(d)$.

Proof. The operator a^*a is positive, hence $\sigma(a^*a) \subset [0, +\infty[$. Let $f(\lambda) = \lambda^{\frac{1}{2}}$ ($\lambda \in \sigma(a^*a)$) and put $d = f(a^*a)$. Since $f = \bar{g}g$, where $g(\lambda) = \lambda^{\frac{1}{4}}$ ($\lambda \in \sigma(a^*a)$), we have $d = g(a^*a)^*g(a^*a)$, so d is positive.

For any $\xi \in \mathcal{H}$ we have

$$\|d\xi\|^2 = \langle d\xi | d\xi \rangle = \langle \xi | d^*d\xi \rangle = \langle \xi | d^2\xi \rangle = \langle \xi | a^*a\xi \rangle = \langle a\xi | a\xi \rangle = \|a\xi\|^2$$

which implies that the mapping

$$\text{ran } d \ni d\xi \longmapsto a\xi \in \mathcal{H}$$

is well-defined and isometric. Consequently we can extend it uniquely to an isometry $v_0: \overline{\text{ran } d} \rightarrow \mathcal{H}$ (with range equal to $\overline{\text{ran } a}$) and define $v \in B(\mathcal{H})$ by

$$v\xi = \begin{cases} v_0\xi & \xi \in \overline{\text{ran } d} \\ 0 & \xi \in (\text{ran } d)^\perp \end{cases}.$$

One easily checks¹ that

$$v^*\eta = \begin{cases} v_0^{-1}\eta & \eta \in \overline{\text{ran } a} \\ 0 & \eta \in (\text{ran } a)^\perp \end{cases},$$

so v^*v is the projection onto $\overline{\text{ran } d}$, i.e. $v^*v = s(d)$. This shows that the pairs (v, d) as in the statement of the theorem exists.

Let $(u, k) \in B(\mathcal{H}) \times B(\mathcal{H})$ be such that

- $a = uk$,
- k is positive,
- $u^*u = s(k)$.

Then $d^2 = a^*a = ku^*uk = k^2$, so defining g to be the function $\lambda \mapsto \lambda^2$ on $\sigma(d)$ and h to be the same function on $\sigma(k)$ we obtain

$$d = f(g(d)) = f(d^2) = f(k^2) = f(h(k)) = k$$

because $f \circ g$ is the identity function on $\sigma(d)$ and $f \circ h$ is the identity on $\sigma(k)$ (note that $\sigma(g(d)) = \sigma(d^2) = \sigma(k^2) = \sigma(h(k))$).

Now u is a partial isometry which satisfies

$$u\xi = \begin{cases} v\xi & \xi \in \overline{\text{ran } d} \\ 0 & \xi \in (\text{ran } d)^\perp \end{cases},$$

since for $\xi \in \overline{\text{ran } d} = \overline{\text{ran } k}$ we have $u\xi = uk\eta = a\eta = v d\eta = vk\eta = v\xi$, so by continuity $u = v$ on $\overline{\text{ran } d}$. Also $u^*u = 0$ on $(\text{ran } k)^\perp = (\text{ran } d)^\perp$ and hence² $u = 0$ on $(\text{ran } d)^\perp$. Consequently $u = v$. \square

The positive part of the polar decomposition of $\text{ain } B(\mathcal{H})$ is called the *absolute value* or the *modulus* of a and it is denoted by $|a|$. Thus $a = v|a|$, where $|a| = (a^*a)^{\frac{1}{2}}$ and $v^*v = s(|a|)$.

2. UNBOUNDED OPERATORS

2.1. Domains, graphs and closures.

An (unbounded) operator T on a Hilbert space \mathcal{H} is a linear mapping

$$\text{Dom}(T) \longrightarrow \mathcal{H},$$

where $\text{Dom}(T)$ is a subspace of \mathcal{H} called the *domain* of T .

Example. Consider the Hilbert space $L_2([0, 1])$ and put

$$\text{Dom}(\partial) = \left\{ \psi \in L_2([0, 1]) \mid \exists \alpha \in \mathbb{C}, \varphi \in L_2([0, 1]) \ \forall x \in [0, 1] \psi(x) = \alpha + \int_0^x \varphi(t) dt \right\}.$$

It turns out that given $\psi \in \text{Dom}(\partial)$ the constant α and $\varphi \in L_2([0, 1])$ such that $\psi(x) = \alpha + \int_0^x \varphi(t) dt$ for almost all $x \in [0, 1]$ are unique and depend linearly on ψ . We define the operator ∂ by $\partial\psi = \varphi$.

¹Take $\psi, \varphi \in \mathcal{H}$ and write $\psi = \psi_1 + \psi_2$ with $\psi_1 \in \overline{\text{ran } a}$, $\psi_2 \in (\text{ran } a)^\perp$ and $\varphi = \varphi_1 + \varphi_2$ with $\varphi_1 \in \overline{\text{ran } d}$, $\varphi_2 \in (\text{ran } d)^\perp$. v_0 is an isometry from $\overline{\text{ran } d}$ onto $\overline{\text{ran } a}$, so

$$\begin{aligned} \langle \psi | v\varphi \rangle &= \langle \psi_1 + \psi_2 | v_0\varphi_1 \rangle = \langle \psi_1 | v_0\varphi_1 \rangle + \underbrace{\langle \psi_2 | v_0\varphi_1 \rangle}_{=0} \\ &= \langle v_0v_0^{-1}\psi_1 | v_0\varphi_1 \rangle \\ &= \langle v_0^{-1}\psi_1 | \varphi_1 \rangle \\ &= \langle v_0^{-1}\psi | \varphi \rangle. \end{aligned}$$

²For any $a \in B(\mathcal{H})$ we have $\ker a = \ker a^*a$.

Note that for $n \in \mathbb{N}$ the function $\psi_n(x) = \sqrt{2n+1}x^n$ ($x \in [0, 1]$) belongs to $\text{Dom}(\partial)$ (since $\psi_n(x) = 0 + \sqrt{2n+1}n \int_0^x t^{n-1} dt$) and $\|\psi_n\|_2 = 1$, but

$$\|\partial\psi_n\|_2^2 = (2n+1)n^2 \int_0^1 x^2 n - 2 dx = n^2 \frac{2n+1}{2n-1} \xrightarrow{n \rightarrow \infty} +\infty.$$

Terminology 3. Let T be an operator on \mathcal{H} .

- T is *densely defined* if $\text{Dom}(T)$ is dense in \mathcal{H} ,
- The *graph* of T is

$$\text{Graph}(T) = \left\{ \begin{bmatrix} \psi \\ T\psi \end{bmatrix} \mid \psi \in \text{Dom}(T) \right\} \subset \mathcal{H} \oplus \mathcal{H},$$

- T is *closed* if $\text{Graph}(T)$ is a closed subspace of the Hilbert space $\mathcal{H} \oplus \mathcal{H}$,
- T is *closable* if $\overline{\text{Graph}(T)}$ is a graph of an operator,
- if T is closable then the operator whose graph is $\overline{\text{Graph}(T)}$ is called the *closure* of T and it is denoted by \overline{T} ,
- and operator S is an *extension* of T is $\text{Graph}(T) \subset \text{Graph}(S)$.

Example. Consider again the operator ∂ on $L_2([0, 1])$. It turns out that ∂ is closed. Note that $\text{Dom}(\partial)$ is contained in $C([0, 1])$ and contains $C^1([0, 1])$ (and for $f \in C^1([0, 1])$ we have $\partial f = f'$). In particular ∂ is densely defined and it makes sense to write

$$\text{Dom}(\partial_{0,0}) = \{\varphi \in \text{Dom}(\partial) \mid \varphi(0) = 0 = \varphi(1)\}, \quad \partial_{0,0} = \partial|_{\text{Dom}(\partial_{0,0})}.$$

Clearly ∂ is an extension of $\partial_{0,0}$. Moreover $\partial_{0,0}$ is closed because

$$\text{Graph}(\partial_{0,0}) = \text{Graph}(\partial) \cap \left\{ \begin{bmatrix} 1 \\ x \end{bmatrix} \right\}^\perp \cap \left\{ \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}^\perp.$$

Fact. Let T be an operator on \mathcal{H}

- (1) T is closed if and only if

$$\left(\begin{array}{c} \psi_n \in \text{Dom}(T) \\ \psi_n \xrightarrow{n \rightarrow \infty} \psi \\ T\psi_n \xrightarrow{n \rightarrow \infty} \varphi \end{array} \right) \implies \left(\begin{array}{c} \psi \in \text{Dom}(T) \\ T\psi = \varphi \end{array} \right).$$

- (2) T is closable if and only if

$$\left(\begin{array}{c} \psi_n \in \text{Dom}(T) \\ \psi_n \xrightarrow{n \rightarrow \infty} 0 \\ T\psi_n \xrightarrow{n \rightarrow \infty} \varphi \end{array} \right) \implies (\varphi = 0).$$

2.2. The spectrum.

In what follows for an unbounded operator T on \mathcal{H} and a number $\lambda \in \mathbb{C}$ we define $\lambda\mathbb{1} - T$ as the operator with domain $\text{Dom}(\lambda\mathbb{1} - T) = \text{Dom}(T)$ acting as $(\lambda\mathbb{1} - T)\psi = \lambda\psi - T\psi$ for $\psi \in \text{Dom}(\lambda\mathbb{1} - T)$. Clearly if T is densely defined then $\lambda\mathbb{1} - T$ is densely defined as well. Moreover, it can be easily shown that $\lambda\mathbb{1} - T$ is closed if T is.

Definition. Let T be a closed, densely defined operator. We say that T is *invertible* if T is a bijection from $\text{Dom}(T)$ onto \mathcal{H} . The *spectrum* of T is

$$\sigma(T) = \{\lambda \in \mathbb{C} \mid T \text{ is not invertible}\}.$$

Remark. It follows from the closed graph theorem that if T is closed and bijective from $\text{Dom}(T)$ onto \mathcal{H} then the inverse map $T^{-1}: \mathcal{H} \rightarrow \text{Dom}(T)$ is bounded.

Theorem. Let T be closed and densely defined. Then $\sigma(T)$ is a closed subset of \mathbb{C} .

Example. We have $\sigma(\partial) = \mathbb{C}$ because for any $\lambda \in \mathbb{C}$ the function $\psi_\lambda(x) = e^{\lambda x}$ ($x \in [0, 1]$) satisfies $\partial\psi_\lambda = \lambda\psi_\lambda$.

Example. Define $\text{Dom}(\partial_0) = \{\varphi \in \text{Dom}(\partial) \mid \varphi(0) = 0\}$ and $\partial_0 = \partial|_{\text{Dom}(\partial_0)}$. Then ∂_0 is closed (and densely defined) and $\sigma(\partial_0) = \emptyset$.

Indeed, defining for $\lambda \in \mathbb{C}$ the operator r_λ by

$$(r_\lambda\psi)(x) = - \int_0^x e^{\lambda(x-t)}\psi(t) dt, \quad \psi \in \text{L}_2([0, 1]), x \in [0, 1]$$

we easily find that $r_\lambda \in \text{B}(\text{L}_2([0, 1]))$ (in fact r_λ is compact) and

- (1) for any $\psi \in \text{L}_2([0, 1])$ we have $r_\lambda\psi \in \text{Dom}(\partial_0)$,
- (2) $(\lambda\mathbf{1} - \partial_0)r_\lambda\psi = \psi$ for any $\psi \in \text{L}_2([0, 1])$,
- (3) $r_\lambda(\lambda\mathbf{1} - \partial_0)\varphi = \varphi$ for any $\varphi \in \text{Dom}(\partial_0)$.

It follows that $\lambda\mathbf{1} - \partial_0$ is invertible for any $\lambda \in \mathbb{C}$ and $\lambda \mapsto r_\lambda$ is the resolvent of ∂_0 .

Example. Fix $\kappa \in [0, 2\pi[$ and let $\mu = e^{i\kappa}$. Define the operator P_μ on $\text{L}_2([0, 1])$ by

$$\text{Dom}(P_\mu) = \{\psi \in \text{Dom}(\partial) \mid \psi(1) = \mu\psi(0)\}$$

and

$$P_\mu\psi = \frac{1}{i}\partial\psi, \quad \psi \in \text{Dom}(P_\mu).$$

Then for all $n \in \mathbb{Z}$ the function $\psi_n(x) = e^{i(2\pi n + \kappa)x}$ ($x \in [0, 1]$) belongs to $\text{Dom}(P_\mu)$ and $P_\mu\psi_n = (2\pi n + \kappa)\psi_n$, so $2\pi\mathbb{Z} + \kappa \subset \sigma(P_\mu)$. It can be shown that $\sigma(P_\mu) = 2\pi\mathbb{Z} + \kappa$.

2.3. The adjoint operator.

Proposition. *Let T be a densely defined operator. Then*

$$\left\{ \begin{bmatrix} \xi \\ \eta \end{bmatrix} \mid \forall \psi \in \text{Dom}(T) \quad \langle \xi | T\psi \rangle = \langle \eta | \psi \rangle \right\}$$

is a graph of a closed operator T^* . Moreover

- (1) $\text{Graph}(T^*) = \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Graph}(T)^\perp$,
- (2) T^* is densely defined if and only if T is closable,
- (3) if T^* is densely defined then $(T^*)^* = \overline{T}$.

Proof. If $\begin{bmatrix} 0 \\ \eta \end{bmatrix} \in \left\{ \begin{bmatrix} \xi \\ \eta \end{bmatrix} \mid \forall \psi \in \text{Dom}(T) \quad \langle \xi | T\psi \rangle = \langle \eta | \psi \rangle \right\}$ then $\langle \eta | \psi \rangle = 0$ for all $\psi \in \text{Dom}(T)$, so $\eta = 0$. This defines T^* .

Next we note that

$$\begin{aligned} \left(\begin{bmatrix} \xi \\ \eta \end{bmatrix} \in \text{Graph}(T^*) \right) &\iff \left(\forall \psi \in \text{Dom}(T) \quad \left\langle \begin{bmatrix} \xi \\ \eta \end{bmatrix} \mid \begin{bmatrix} T\psi \\ -\psi \end{bmatrix} \right\rangle = 0 \right) \\ &\iff \left(\begin{bmatrix} \xi \\ \eta \end{bmatrix} \perp \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Graph}(T) \right) \\ &\iff \left(\begin{bmatrix} \xi \\ \eta \end{bmatrix} \in \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Graph}(T)^\perp \right) \end{aligned}$$

which also shows that T^* is closed.

The operator T is closable if and only if $\overline{\text{Graph}(T)}$ does not contain non-zero vectors of the form $\begin{bmatrix} 0 \\ \varphi \end{bmatrix}$. Note further that the formula $\text{Graph}(T^*) = \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Graph}(T)^\perp$ implies that

$$\text{Graph}(T^*)^\perp = \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \overline{\text{Graph}(T)},$$

so T is closable if and only if $\text{Graph}(T^*)^\perp$ does not contain non-zero vectors of the form $\begin{bmatrix} \varphi \\ 0 \end{bmatrix}$ which is equivalent to $\text{Dom}(T^*) = \left\{ \xi \in \mathcal{H} \mid \exists \eta \begin{bmatrix} \xi \\ \eta \end{bmatrix} \in \text{Graph}(T^*) \right\}$ being dense in \mathcal{H} .

Finally

$$\text{Graph}(\overline{T}) = \overline{\text{Graph}(T)} = \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Graph}(T^*)^\perp = \text{Graph}((T^*)^*).$$

□

Definition. The operator T^* defined in the theorem above is called the *adjoint* of T .

Corollary. Let T be a densely defined operator and S an extension of T . Then $T^* \supset S^*$.

Definition. An operator T is called *symmetric* or *hermitian* if $T \subset T^*$. We has that T is *self-adjoint* if $T = T^*$.

Proposition.

(1) An operator T is symmetric if and only if for any $\varphi, \psi \in \text{Dom}(T)$ we have

$$\langle \varphi | T\psi \rangle = \langle T\varphi | \psi \rangle, \quad (2)$$

(2) a self-adjoint operator has no proper symmetric extensions.

Proof. The first statement is almost obvious, since (2) means precisely that any $\varphi \in \text{Dom}(T)$ belongs to $\text{Dom}(T^*)$ and $T^*\varphi = T\varphi$.

As for the second statement, take a symmetric S such that $T \subset S$. Then $T^* \supset S$, so

$$T = T^* \supset S^* \supset S \supset T,$$

and consequently $T = S$. □

Example. Let $T = \frac{1}{i}\partial_{0,0}$ on $L_2([0,1])$. Then $T^* = \frac{1}{i}\partial$. The fact that $\frac{1}{i}\partial \subset T^*$ follows from the calculation: for $\varphi \in \text{Dom}(T) = \text{Dom}(\partial_{0,0})$ and $\psi \in \text{Dom}(\partial)$

$$\begin{aligned} \langle \varphi | T\psi \rangle &= \int_0^1 \overline{\varphi(t)} \frac{1}{i} (\partial\psi)(t) dt \\ &= \frac{1}{i} \left(\overline{\varphi(1)} \underbrace{\psi(1)}_{=0} - \overline{\varphi(0)} \underbrace{\psi(0)}_{=0} - \int_0^1 (\partial\varphi)(t) \psi(t) dt \right) \\ &= -\frac{1}{i} \langle \partial\varphi | \psi \rangle = \langle \frac{1}{i}\partial\varphi | \psi \rangle. \end{aligned}$$

The converse inclusion requires some more involved approximations.

We also have

- $T \subset \frac{1}{i}\partial$, so that T is symmetric, but not self-adjoint,
- since T is closed, we have $(\frac{1}{i}\partial)^* = T$.

Example. Put $T_0 = \frac{1}{i}\partial_0$ (recall $\text{Dom}(\partial_0) = \{\varphi \in \text{Dom}(\partial) \mid \varphi(0) = 0\}$, $\partial_0 = \partial|_{\text{Dom}(\partial_0)}$) and $T_1 = \frac{1}{i}\partial_1$ with $\text{Dom}(\partial_1) = \{\varphi \in \text{Dom}(\partial) \mid \varphi(1) = 0\}$ and $\partial_1 = \partial|_{\text{Dom}(\partial_1)}$. Then $T_0^* = T_1$ (and $T_1^* = T_0$).

Example. For any $\mu \in \mathbb{T}$ the operator P_μ is self-adjoint. Note that each P_μ is an extension of $\frac{1}{i}\partial_{0,0}$.

2.4. Algebraic operators.

Given two operators T and S on \mathcal{H} we define

$$\begin{aligned}\text{Dom}(TS) &= \{\psi \in \text{Dom}(S) \mid S\psi \in \text{Dom}(T)\}, \\ \text{Dom}(T + S) &= \text{Dom}(T) \cap \text{Dom}(S)\end{aligned}$$

and $TS\psi = T(S\psi)$ ($\psi \in \text{Dom}(TS)$), $(T + S)\varphi = T\varphi + S\varphi$ ($\varphi \in \text{Dom}(T + S)$).

Even when T and S are densely defined and closed the operators TS and $T + S$ might fail to be densely defined or closed (or closable).

Proposition. *Let S and T be closed and densely defined operators and let $a \in \text{B}(\mathcal{H})$, Then*

- (1) $T + a$ is closed,
- (2) Ta is closed,
- (3) if a is invertible (in $\text{B}(\mathcal{H})$) then aT is closed,
- (4) if TS is densely defined then $S^*T^* \subset (TS)^*$,
- (5) $(aT)^* = T^*a^*$,
- (6) if $T + S$ is densely defined then $T^* + S^* \subset (T + S)^*$,
- (7) $(T + a)^* = T^* + a^*$.

We say that an operator T on \mathcal{H} is *positive* if $\langle \psi | T\psi \rangle \geq 0$ for all $\psi \in \text{Dom}(T)$. A positive operator is symmetric, but may fail to be self-adjoint (when it is not bounded).

Fact. Let T be a closed and densely defined operator. Then the operator T^*T is

- closed,
- densely defined,
- positive,
- self-adjoint.

Example. Let $S = T^2$, where $T = \frac{1}{i}\partial_{0,0}$ as in several examples above), i.e.

$$\text{Dom}(S) = \{\varphi \in \text{Dom}(\partial_{0,0}) \mid \partial\varphi \in \text{Dom}(\partial_{0,0})\}$$

and

$$S\varphi = -\partial^2\varphi, \quad \varphi \in \text{Dom}(S).$$

Then S is

- positive,
- closed,
- not self-adjoint.

3. THE z -TRANSFORM OF A CLOSED DENSELY DEFINED OPERATOR

3.1. Definition of the z -transform.

Theorem. *Let T be a closed densely defined operator on a Hilbert space \mathcal{H} . Then the mapping*

$$\text{Dom}(T^*T) \ni \psi \longmapsto \psi + T^*T\psi$$

is a bijection not decreasing the norm.

Proof. Recall that

$$\text{Graph}(T)^\perp = \begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Graph}(T^*) = \left\{ \begin{bmatrix} T^*\varphi \\ -\varphi \end{bmatrix} \mid \varphi \in \text{Dom}(T^*) \right\}.$$

Since $\mathcal{H} \oplus \mathcal{H} = \text{Graph}(T) \oplus \text{Graph}(T)^\perp$, for any $\xi, \eta \in \mathcal{H}$ there are $\psi \in \text{Dom}(T)$ and $\varphi \in \text{Dom}(T^*)$ such that

$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} \psi \\ T\psi \end{bmatrix} + \begin{bmatrix} T^*\varphi \\ -\varphi \end{bmatrix}.$$

Setting $\eta = 0$, we obtain

$$\forall \xi \in \mathcal{H} \quad \exists \psi \in \text{Dom}(T), \varphi \in \text{Dom}(T^*) \quad \begin{bmatrix} \xi \\ 0 \end{bmatrix} = \begin{bmatrix} \psi \\ T\psi \end{bmatrix} + \begin{bmatrix} T^*\varphi \\ -\varphi \end{bmatrix},$$

i.e.

$$\forall \xi \in \mathcal{H} \exists \psi \in \text{Dom}(T^*T) \quad \xi = \psi + T^*T\psi.$$

Furthermore once $\xi = \psi + T^*T\psi$ for some $\psi \in \text{Dom}(T^*T)$ then

$$\|\xi\|^2 = \langle \psi + T^*T\psi | \psi + T^*T\psi \rangle = \|\psi\|^2 + 2\|T\psi\|^2 + \|T^*T\psi\|^2 \geq \|\psi\|^2.$$

Consequently, if $\psi + T^*T\psi = \psi' + T^*T\psi'$ for $\psi, \psi' \in \text{Dom}(T^*T)$ then

$$0 = (\psi - \psi') + T^*T(\psi - \psi'),$$

so $0 = \|0\|^2 \geq \|\psi - \psi'\|^2$. □

Consider a closed and densely defined operator T on \mathcal{H} . The inverse $(\mathbf{1} + T^*T)^{-1}$ of the bijection $\mathbf{1} + T^*T: \text{Dom}(T^*T) \rightarrow \mathcal{H}$ is contractive and hence bounded (and consequently closed). It follows that $\mathbf{1} + T^*T$ is closed, so that also $T^*T = (\mathbf{1} + T^*T) + (-\mathbf{1})$ is closed.

Suppose $\begin{bmatrix} \psi \\ T\psi \end{bmatrix} \in \text{Graph}(T)$ is orthogonal to $\text{Graph}(T|_{\text{Dom}(T^*T)})$:

$$\forall \varphi \in \text{Dom}(T^*T) \quad \left\langle \begin{bmatrix} \psi \\ T\psi \end{bmatrix} \middle| \begin{bmatrix} \varphi \\ T\varphi \end{bmatrix} \right\rangle = 0.$$

Then $\langle \psi | \varphi \rangle + \langle T\psi | T\varphi \rangle = 0$ for all $\varphi \in \text{Dom}(T^*T)$, i.e.

$$\forall \varphi \in \text{Dom}(T^*T) \quad \psi \perp (\mathbf{1} + T^*T)\varphi.$$

In other words $\psi \perp \mathcal{H}$, so that $\psi = 0$. It follows that $\text{Graph}(T|_{\text{Dom}(T^*T)})$ is dense in $\text{Graph}(T)$:

$$T = \overline{T|_{\text{Dom}(T^*T)}}.$$

In particular $\text{Dom}(T^*T)$ is dense in \mathcal{H} (it is a *core* for T).

Lemma. *The operator $(\mathbf{1} + T^*T)^{-1}$ is positive.*

Proof. Take $\xi \in \mathcal{H}$ and put $\psi = (\mathbf{1} + T^*T)^{-1}\xi \in \text{Dom}(T^*T)$. Then

$$\langle \xi | (\mathbf{1} + T^*T)^{-1}\xi \rangle = \langle \xi | \psi \rangle = \langle (\mathbf{1} + T^*T)\psi | \psi \rangle = \|\psi\|^2 + \|T\psi\|^2 \geq 0.$$

□

We will denote by $(\mathbf{1} + T^*T)^{-\frac{1}{2}}$ the square root of the positive operator $(\mathbf{1} + T^*T)^{-1}$, i.e. $(\mathbf{1} + T^*T)^{-\frac{1}{2}} = f((\mathbf{1} + T^*T)^{-1})$, where f is the function $\lambda \mapsto \lambda^{\frac{1}{2}}$ on $\sigma((\mathbf{1} + T^*T)^{-1})$.

Theorem. *Let T be a closed densely defined operator. Then*

- (1) $\text{ran}(\mathbf{1} + T^*T)^{-\frac{1}{2}} = \text{Dom}(T)$,
- (2) $T(\mathbf{1} + T^*T)^{-\frac{1}{2}} \in \mathcal{B}(\mathcal{H})$ and $\|(\mathbf{1} + T^*T)^{-\frac{1}{2}}\| \leq 1$.

Definition. Let T be a closed densely defined operator. The bounded operator $z_T = T(\mathbf{1} + T^*T)^{-\frac{1}{2}}$ is called the *z-transform* of T .

Remark. Since $\|z_T\| \leq 1$, we have $0 \leq z_T^*z_T \leq \mathbf{1}$, so in particular $\mathbf{1} - z_T^*z_T$ is positive (similarly $\mathbf{1} - z_Tz_T^*$ is positive).

3.2. Properties of the z-transform.

Theorem. *Let T be a closed densely defined operator. Then*

$$\text{Graph}(T) = \left\{ \left[\begin{array}{c} (\mathbf{1} + z_T^*z_T)^{\frac{1}{2}}\xi \\ z_T\xi \end{array} \right] \middle| \xi \in \mathcal{H} \right\}.$$

Proof. Since $\text{Dom}(T) = \text{ran}(\mathbf{1} + T^*T)^{-\frac{1}{2}}$, we have

$$\begin{aligned} \text{Graph}(T) &= \left\{ \begin{bmatrix} \psi \\ T\psi \end{bmatrix} \mid \psi \in \text{Dom}(T) \right\} \\ &= \left\{ \begin{bmatrix} (\mathbf{1} + T^*T)^{-\frac{1}{2}}\xi \\ T(\mathbf{1} + T^*T)^{-\frac{1}{2}}\xi \end{bmatrix} \mid \xi \in \mathcal{H} \right\} \\ &= \left\{ \begin{bmatrix} (\mathbf{1} + T^*T)^{-\frac{1}{2}}\xi \\ z_T\xi \end{bmatrix} \mid \xi \in \mathcal{H} \right\} \end{aligned}$$

and it remains to prove that $(\mathbf{1} + T^*T)^{-\frac{1}{2}} = (\mathbf{1} - z_T^*z_T)^{\frac{1}{2}}$ or that

$$(\mathbf{1} + T^*T)^{-1} = (\mathbf{1} - z_T^*z_T). \quad (3)$$

Take $\xi \in \mathcal{H}$ and let $\psi = (\mathbf{1} + T^*T)^{-\frac{1}{2}}\xi$. We have

$$\begin{aligned} \|\psi\|^2 &= \left\langle (\mathbf{1} + T^*T)^{-\frac{1}{2}}\xi \mid (\mathbf{1} + T^*T)^{-\frac{1}{2}}\xi \right\rangle \\ &= \langle \xi \mid (\mathbf{1} + T^*T)^{-1}\xi \rangle \\ &= \langle (\mathbf{1} + T^*T)(\mathbf{1} + T^*T)^{-1}\xi \mid (\mathbf{1} + T^*T)^{-1}\xi \rangle \\ &= \|(\mathbf{1} + T^*T)^{-1}\xi\|^2 + \langle T^*T(\mathbf{1} + T^*T)^{-1}\xi \mid (\mathbf{1} + T^*T)^{-1}\xi \rangle \\ &= \|(\mathbf{1} + T^*T)^{-1}\xi\|^2 + \langle T(\mathbf{1} + T^*T)^{-1}\xi \mid T(\mathbf{1} + T^*T)^{-1}\xi \rangle \\ &= \|(\mathbf{1} + T^*T)^{-\frac{1}{2}}\psi\|^2 + \|z_T\psi\|^2. \end{aligned}$$

Hence, by continuity we obtain $\|\psi\|^2 = \|(\mathbf{1} + T^*T)^{-\frac{1}{2}}\psi\|^2 + \|z_T\psi\|^2$ for all $\psi \in \mathcal{H}$.

In other words the sesquilinear forms

$$(\psi, \varphi) \longmapsto \langle (\mathbf{1} + T^*T)^{-\frac{1}{2}}\psi \mid (\mathbf{1} + T^*T)^{-\frac{1}{2}}\varphi \rangle \quad \text{and} \quad (\psi, \varphi) \longmapsto \langle \psi \mid \varphi \rangle - \langle z_T\psi \mid z_T\varphi \rangle,$$

i.e. the forms

$$(\psi, \varphi) \longmapsto \langle \psi \mid (\mathbf{1} + T^*T)^{-1}\varphi \rangle \quad \text{and} \quad (\psi, \varphi) \longmapsto \langle \psi \mid (\mathbf{1} - z_T^*z_T)\varphi \rangle$$

coincide when $\varphi = \psi$. Thus, by polarization, they are equal, and we obtain (3). \square

It follows from the theorem above that z_T contains the full information about T :

Corollary. *Let S and T be closed densely defined operators. If $z_S = z_T$ then $S = T$.*

Example. Consider $\mathcal{H} = L_2([0, 1])$ and $T = \frac{1}{i}\partial_{0,0}$, so that $T^*T = -\Delta_D$ (the Dirichlet Laplacian). For $n \in \mathbb{N}$ let

$$s_n(x) = \sqrt{2} \sin(\pi nx), \quad x \in [0, 1].$$

Then $(s_n)_{n \in \mathbb{N}}$ is an orthonormal basis of \mathcal{H} and $T^*T s_n = \pi^2 n^2 s_n$ for all n . It follows that $(\mathbf{1} - T^*T)^{-\frac{1}{2}} s_n = (\mathbf{1} + \pi^2 n^2)^{-\frac{1}{2}} s_n$ and consequently with

$$c_n(x) = \sqrt{2} \cos(\pi nx), \quad x \in [0, 1], \quad n \in \mathbb{Z}_+$$

we obtain³

$$z_T s_n = \frac{\pi n}{\sqrt{1 + \pi^2 n^2}} c_n = \sum_{m=1}^{\infty} \frac{2nm(1 - (-1)^{m+n})}{\sqrt{1 + \pi^2 n^2}(m^2 - n^2)} s_m, \quad n \in \mathbb{N}.$$

³The expansion of c_n in the basis $(s_m)_{m \in \mathbb{N}}$ is found by calculating the scalar products

$$\langle s_m \mid c_n \rangle = 2 \int_0^1 \sin(\pi mx) \cos(\pi nx) dx = \frac{2m}{\pi(m^2 - n^2)} (1 - (-1)^{m+n}).$$

While the above expression is not very helpful in the analysis of T , we nevertheless see that the domain of T (which is equal to the range of $(\mathbb{1} + T^*T)^{-\frac{1}{2}}$) can be described as those vectors $\psi \in \mathbf{L}_2([0, 1])$ whose expansion

$$\psi = \sum_{n=1}^{\infty} \alpha_n s_n$$

in the basis $(s_n)_{n \in \mathbb{N}}$ satisfies $\sum_{n=1}^{\infty} n^2 |\alpha_n|^2 < +\infty$. In particular the series $\sum_{n=1}^{\infty} \alpha_n s_n$ is uniformly convergent.⁴

Remark. We have $\ker(\mathbb{1} - z_T^* z_T) = \{0\}$. Indeed, $\ker(\mathbb{1} - z_T^* z_T) = \text{ran}(\mathbb{1} - z_T^* z_T)^\perp$ and since $\mathbb{1} - z_T^* z_T = (\mathbb{1} + T^*T)^{-1}$ is a bijection $\text{Dom}(T^*T) \rightarrow \mathcal{H}$, we see that $\text{ran}(\mathbb{1} - z_T^* z_T)^\perp = \text{Dom}(T^*T)^\perp = \{0\}$.

Theorem. *The assignment $T \mapsto z_T$ establishes a bijection from the set of closed densely defined operators on \mathcal{H} onto the set $\{z \in \mathbf{B}(\mathcal{H}) \mid \|z\| \leq 1, \ker(\mathbb{1} - z^*z) = \{0\}\}$.*

Remark. Note that if $z \in \mathbf{B}(\mathcal{H})$ is such that $\ker(\mathbb{1} - z^*z) = \{0\}$ then also $\ker(\mathbb{1} - zz^*) = \{0\}$. Indeed, is $(\mathbb{1} - zz^*)\varphi = 0$ then $z^*(\mathbb{1} - zz^*)\varphi = 0$, i.e. $(\mathbb{1} - z^*z)z^*\varphi = 0$ which implies $z^*\varphi = 0$. But this reduces $(\mathbb{1} - zz^*)\varphi = 0$ to $\varphi = 0$.

Proposition. *Let $\mathcal{H}_{\text{HOR}} = \left\{ \begin{bmatrix} \xi \\ 0 \end{bmatrix} \mid \xi \in \mathcal{H} \right\}$. Then for any closed densely defined operator T we have $\text{Graph}(T) = U_T(\mathcal{H}_{\text{HOR}})$, where*

$$U_T = \begin{bmatrix} (\mathbb{1} - z_T^* z_T)^{\frac{1}{2}} & -z_T^* \\ z_T & (\mathbb{1} - z_T z_T^*)^{\frac{1}{2}} \end{bmatrix}$$

is a unitary operator on $\mathcal{H} \oplus \mathcal{H}$.

Corollary. $\text{Graph}(T)^\perp = \left\{ \begin{bmatrix} -z_T^* \xi \\ (\mathbb{1} - z_T z_T^*)^{\frac{1}{2}} \xi \end{bmatrix} \mid \xi \in \mathcal{H} \right\}$.

Proof. We have

$$\text{Graph}(T)^\perp = \left(U_T(\mathcal{H}_{\text{HOR}}) \right)^\perp = U_T(\mathcal{H}_{\text{HOR}}^\perp) = U_T(\mathcal{H}_{\text{VERT}}),$$

where $\mathcal{H}_{\text{VERT}} = \left\{ \begin{bmatrix} 0 \\ \eta \end{bmatrix} \mid \eta \in \mathcal{H} \right\}$. □

Corollary. $z_{T^*} = z_T^*$.

Proof. We have

$$\text{Graph}(T^*) = \begin{bmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{bmatrix} \text{Graph}(T)^\perp = \left\{ \begin{bmatrix} (\mathbb{1} - z_T z_T^*)^{\frac{1}{2}} \xi \\ z_T^* \xi \end{bmatrix} \mid \xi \in \mathcal{H} \right\}$$

which shows that the operator whose z -transform is z_T^* coincides with T^* . □

3.3. Polar decomposition of closed operators.

Theorem. *Let T be a closed densely defined operator on \mathcal{H} . Then there exists a unique pair (u, K) such that*

- K is a positive self-adjoint operator on \mathcal{H} ,
- $u \in \mathbf{B}(\mathcal{H})$ is such that u^*u is the projection onto $\overline{\text{ran } K}$,
- $T = uK$

Remark. Let T, u and K be as above. Then u enters the polar decomposition of z_T : $z_T = u|z_T|$ while $z_K = |z_T|$.

⁴We have $\sum_{n=1}^{\infty} |\alpha_n| = \sum_{n=1}^{\infty} (n|\alpha_n|)^{\frac{1}{n}} \leq \left(\sum_{n=1}^{\infty} n^2 |\alpha_n|^2 \right)^{\frac{1}{2}} \left(\sum_{n=1}^{\infty} \frac{1}{n^2} \right)^{\frac{1}{2}} < +\infty$, so the series converges uniformly by Weierstrass test.

3.4. Functional calculus.

Define $\zeta: \mathbb{R} \rightarrow]-1, 1[$ by

$$\zeta(x) = \frac{x}{\sqrt{1+x^2}}, \quad x \in \mathbb{R}.$$

Theorem. *Let T be a self-adjoint operator on \mathcal{H} . Then there exists a unique unital $*$ -homomorphism $C_b(\mathbb{R}) \rightarrow B(\mathcal{H})$ denoted by $f \mapsto f(T)$ such that $\zeta(T) = z_T$.*

4. SELF-ADJOINT EXTENSIONS OF SYMMETRIC OPERATORS

4.1. The Cayley transform.

Remark. A symmetric operator T is always closable (since $T \subset T^*$ the latter is densely defined). Moreover \overline{T} is symmetric (because T^* is closed). Consequently any self-adjoint extension of a symmetric operator T is an extension of \overline{T} .

Proposition. *Let S and T be closed densely defined operators. Then $T \subset S$ if and only if*

$$(\mathbf{1} - z_S z_S^*)^{\frac{1}{2}} z_T = z_S (\mathbf{1} - z_T^* z_T)^{\frac{1}{2}}. \quad (4)$$

Proof. Recall that

$$\text{Graph}(T) = U_T(\mathcal{H}_{\text{HOR}}) \quad \text{and} \quad \text{Graph}(S) = U_S(\mathcal{H}_{\text{HOR}}),$$

where

$$U_T = \begin{bmatrix} (\mathbf{1} - z_T^* z_T)^{\frac{1}{2}} & -z_T^* \\ z_T & (\mathbf{1} - z_T z_T^*)^{\frac{1}{2}} \end{bmatrix}, \quad U_S = \begin{bmatrix} (\mathbf{1} - z_S^* z_S)^{\frac{1}{2}} & -z_S^* \\ z_S & (\mathbf{1} - z_S z_S^*)^{\frac{1}{2}} \end{bmatrix}$$

are unitary operators on $\mathcal{H} \oplus \mathcal{H}$. Now $T \subset S$ if and only if $\text{Graph}(T) \subset \text{Graph}(S)$, i.e.

$$U_T(\mathcal{H}_{\text{HOR}}) \subset U_S(\mathcal{H}_{\text{HOR}}).$$

Acting with U_S^* on both sides of this relation we find that $U_S^* U_T$ preserves the subspace \mathcal{H}_{HOR} , so the lower-left corner of the matrix representation of this operator must be zero. A simple calculation shows that this is equivalent to (4). \square

Corollary. *A closed densely defined operator T is symmetric if and only if*

$$(\mathbf{1} - z_T^* z_T)^{\frac{1}{2}} z_T = z_T^* (\mathbf{1} - z_T z_T^*)^{\frac{1}{2}}.$$

Corollary. *Let T be a closed symmetric operator. Then*

$$w_+ = z_T + i(\mathbf{1} - z_T^* z_T)^{\frac{1}{2}} \quad \text{and} \quad w_- = z_T - i(\mathbf{1} - z_T^* z_T)^{\frac{1}{2}}$$

are isometries.

Put $\mathcal{W}_{\pm} = \text{ran } w_{\pm}$ and $\mathcal{D}_{\pm} = \mathcal{W}_{\pm}^{\perp}$.

Definition. Let T be a closed symmetric operator. The subspaces \mathcal{D}_+ and \mathcal{D}_- are called the *deficiency subspaces* of T and their dimensions $n_{\pm} = \dim \mathcal{D}_{\pm}$ are the *deficiency indices* of T .

Proposition. $\mathcal{D}_{\pm} = \ker(T^* \mp i\mathbf{1})$.

Proof. $\zeta \in \mathcal{D}_{\pm}$ if and only if

$$0 = \langle \zeta | z_T \xi \pm i(\mathbf{1} - z_T^* z_T)^{\frac{1}{2}} \xi \rangle, \quad \xi \in \mathcal{H},$$

so since

$$\text{Graph}(T) = \left\{ \left[\begin{array}{c} (\mathbf{1} + z_T^* z_T)^{\frac{1}{2}} \xi \\ z_T \xi \end{array} \right] \mid \xi \in \mathcal{H} \right\},$$

we find that $\zeta \in \mathcal{D}_{\pm}$ if and only if

$$0 = \langle \zeta | T\psi \pm i\psi \rangle, \quad \psi \in \text{Dom}(T)$$

which means that $\zeta \in \text{Dom}(T^*)$ and $T^* \zeta = \pm i\zeta$. \square

Notation/terminology. If $v \in \mathbf{B}(\mathcal{H})$ is a partial isometry then we denote by \hat{v} the map v restricted to the subspace

$$\text{Dom}(\hat{v}) = \{\xi \in \mathcal{H} \mid \|v\xi\| = \|\xi\|\} = \text{ran } v^*v = (\ker v)^\perp.$$

This subspace is called the *initial subspace* of v , while the range of v is referred to as the *final subspace* of v .

Proposition. Let T be a closed symmetric operator. Then $c_T = w_-w_+^*$ is a partial isometry with initial subspace \mathcal{W}_+ and final subspace \mathcal{W}_- .

Definition. Let T be a closed symmetric operator. The operator c_T° is called the *Cayley transform* of T .

4.2. Self-adjoint extensions.

Theorem. Let T be a closed symmetric operator.

- (1) $\text{Graph}(T) = \begin{bmatrix} -i\mathbf{1} & i\mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{bmatrix} \text{Graph}(c_T^\circ),$
- (2) $\overline{\text{ran}(c_T - \mathbf{1})c_T^*} = \mathcal{H}.$

Proof. Ad (1). We have

$$\begin{aligned} \text{Graph}(c_T^\circ) &= \left\{ \begin{bmatrix} \theta \\ w_-w_+^*\theta \end{bmatrix} \mid \theta \in \mathcal{W}_+ \right\} = \left\{ \begin{bmatrix} w_+\xi \\ w_-\xi \end{bmatrix} \mid \xi \in \mathcal{H} \right\} \\ &= \left\{ \begin{bmatrix} T\psi + i\psi \\ T\psi - i\psi \end{bmatrix} \mid \psi \in \text{Dom}(T) \right\} \\ &= \begin{bmatrix} -i\mathbf{1} & i\mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{bmatrix} \text{Graph}(c_T). \end{aligned}$$

Ad (2). The fact that T is densely defined is equivalent to $\text{Graph}(T)^\perp \cap \mathcal{H}_{\text{HOR}} = \{0\}$. Thus we have

$$\left(\begin{bmatrix} \eta \\ 0 \end{bmatrix} \perp \begin{bmatrix} -i\mathbf{1} & i\mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{bmatrix} \text{Graph}(c_T^\circ) \right) \implies (\eta = 0),$$

i.e.

$$\left(\forall \theta \in \text{Dom}(c_T^\circ) \begin{bmatrix} \eta \\ 0 \end{bmatrix} \perp \begin{bmatrix} -i\mathbf{1} & i\mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{bmatrix} \begin{bmatrix} \theta \\ c_T^\circ\theta \end{bmatrix} \right) \implies (\eta = 0),$$

or in other words

$$\left(\forall \theta \in \text{Dom}(c_T^\circ) \langle \eta \mid (c_T^\circ - \mathbf{1})\theta \rangle = 0 \right) \implies (\eta = 0).$$

Finally we note that $\mathcal{W}_+ = \text{ran } c_T^*$, so the condition

$$\eta \perp \text{ran}(c_T - \mathbf{1})c_T^*$$

implies $\eta = 0$. □

Theorem.

- (1) The assignment $T \mapsto c_T$ is a bijection from the set of closed symmetric operators on \mathcal{H} onto the set of partial isometries $c \in \mathbf{B}(\mathcal{H})$ such that $\text{ran}(c - \mathbf{1})c^* = \mathcal{H}$,
- (2) we have $T_1 \subset T_2$ if and only if $c_{T_1}^\circ \subset c_{T_2}^\circ$,
- (3) T is self-adjoint if and only if c_T is unitary.

Remark. c_T is unitary if and only if $\mathcal{D}_\pm = \{0\}$, i.e. $n_\pm = 0$.

Corollary. A closed symmetric operator has a self-adjoint extension if and only if $n_+ = n_-$. In this case the set of self-adjoint extensions of T is in bijection with the set of unitary operators $\mathcal{D}_+ \rightarrow \mathcal{D}_-$.

Remark. Statement (3) in the theorem above follows from the fact that

$$\text{Graph}(T^*) = \text{Graph}(T) \oplus \tilde{\mathcal{D}}_+ \oplus \tilde{\mathcal{D}}_-,$$

where

$$\tilde{\mathcal{D}}_+ = \left\{ \begin{bmatrix} \xi \\ i\xi \end{bmatrix} \mid \xi \in \mathcal{D}_+ \right\}, \quad \tilde{\mathcal{D}}_- = \left\{ \begin{bmatrix} \eta \\ -i\eta \end{bmatrix} \mid \eta \in \mathcal{D}_- \right\}.$$

Example. Consider $\mathcal{H} = \text{L}_2([0, 1])$ and $T = \frac{1}{i}\partial_{0,0}$ with domain

$$\text{Dom}(T) = \text{Dom}(\partial_{0,0}) = \{\varphi \in \text{Dom}(\partial) \mid \varphi(0) = 0 = \varphi(1)\}.$$

We know that $T^* = \frac{1}{i}\partial$, so $\mathcal{D}_\pm = \{\varphi \in \text{Dom}(\partial) \mid \frac{1}{i}\partial\varphi = \pm i\varphi\}$, i.e. $\mathcal{D}_\pm = \text{span}\{\epsilon_\pm\}$, where

$$\begin{aligned} \epsilon_+(x) &= \sqrt{\frac{2}{e^2-1}}e^{1-x} \\ \epsilon_-(x) &= \sqrt{\frac{2}{e^2-1}}e^x \end{aligned}, \quad x \in [0, 1]$$

(in particular $n_\pm = 1$). Unitary operators $\mathcal{D}_+ \rightarrow \mathcal{D}_-$ are all of the form $\epsilon_+ \mapsto \alpha\epsilon_-$ with $\alpha \in \mathbb{T}$.

Thus the graph of an extension of c_T° to a unitary operator is

$$\text{Graph}(c_T^\circ) \oplus \text{span}\left\{ \begin{bmatrix} \epsilon_+ \\ \alpha\epsilon_- \end{bmatrix} \right\}$$

and the corresponding extension T_α of T is determined by

$$\text{Graph}(T_\alpha) = \begin{bmatrix} -i\mathbb{1} & i\mathbb{1} \\ \mathbb{1} & \mathbb{1} \end{bmatrix} \text{Graph}(c_T^\circ) + \text{span}\left\{ \begin{bmatrix} -i\epsilon_+ + i\alpha\epsilon_- \\ \epsilon_+ + \alpha\epsilon_- \end{bmatrix} \right\}.$$

Note also that

$$\text{span}\left\{ \begin{bmatrix} -i\epsilon_+ + i\alpha\epsilon_- \\ \epsilon_+ + \alpha\epsilon_- \end{bmatrix} \right\} = \text{span}\left\{ \begin{bmatrix} \epsilon_+ - \alpha\epsilon_- \\ i\epsilon_+ + i\alpha\epsilon_- \end{bmatrix} \right\}.$$

In particular $\text{Dom}(T_\alpha) = \text{Dom}(T) + \text{span}\{\epsilon_+ - \alpha\epsilon_-\}$. Thus the values of elements of $\text{Dom}(T_\alpha)$ at the end-points of $[0, 1]$ are determined by the values at 0 and 1 of the function $\epsilon_+ - \alpha\epsilon_-$:

- $(\epsilon_+ - \alpha\epsilon_-)(0) = \sqrt{\frac{2}{e^2-1}}(e - \alpha)$,
- $(\epsilon_+ - \alpha\epsilon_-)(1) = \sqrt{\frac{2}{e^2-1}}(1 - \alpha e)$.

Denote by μ the number

$$\frac{(\epsilon_+ - \alpha\epsilon_-)(1)}{(\epsilon_+ - \alpha\epsilon_-)(0)} = \frac{e - \alpha}{1 - \alpha e} = \frac{-1}{\alpha} \frac{e - \alpha}{e - \alpha} \in \mathbb{T}.$$

Then

$$\text{Dom}(T_\alpha) = \{\varphi \in \text{Dom}(\partial) \mid \varphi(1) = \mu\varphi(0)\}.$$

Note also that the correspondence $\alpha \leftrightarrow \mu$ is bijective:

$$\alpha = \frac{e - \mu}{1 - \mu e}.$$

Finally $T_\alpha(\epsilon_+ - \alpha\epsilon_-) = i\epsilon_+ + i\alpha\epsilon_- = \frac{1}{i}\partial(\epsilon_+ - \alpha\epsilon_-)$, so $T_\alpha = \frac{1}{i}\partial$ on $\text{Dom}(T_\alpha)$ (This is in fact clear from the simple observation that any self-adjoint extension of a symmetric operator is a restriction of its adjoint). In other words $T_\alpha = P_\mu$.

4.3. Von Neumann's theorem.

An operator $J: \mathcal{H} \rightarrow \mathcal{H}$ is *anti-linear* if

- $\forall \xi, \eta \in \mathcal{H} \quad J(\xi + \eta) = J(\xi) + J(\eta)$,
- $\forall \xi \in \mathcal{H}, \alpha \in \mathbb{C} \quad J(\alpha\xi) = \bar{\alpha}J(\xi)$.

As with linear operators, we usually write $J\xi$ instead of $J(\xi)$ for the value of K on ξ .

An anti-linear operator $J: \mathcal{H} \rightarrow \mathcal{H}$ is *anti-unitary* if J is isometric and surjective. One can show that this is equivalent to J being a surjective anti-linear map satisfying

$$\langle J\xi \mid J\eta \rangle = \langle \eta \mid \xi \rangle, \quad \xi, \eta \in \mathcal{H}.$$

Finally we say that an anti-linear operator J is an *anti-unitary involution* if J is anti-unitary and $J^2 = \mathbb{1}$.

Theorem. Let T be a symmetric operator on \mathcal{H} and let J be an anti-unitary involution on \mathcal{H} such that

- $J(\text{Dom}(T)) \subset \text{Dom}(T)$,
- $\forall \psi \in \text{Dom}(T) \quad TJ\psi = JT\psi$.

Then T has a self-adjoint extension.

Ideal of proof. J maps \mathcal{D}_+ bijectively onto \mathcal{D}_- . □

Example. As before let $T = \frac{1}{i}\partial_{0,0}$ on $L_2([0, 1])$. For $\xi \in L_2([0, 1])$ Let $(J\xi)(x) = -\overline{\xi(x)}$ ($x \in [0, 1]$). Clearly J is an anti-unitary involution, $J(\text{Dom}(T)) \subset \text{Dom}(T)$ and for any $\psi \in \text{Dom}(T)$ we have

$$TJ\psi = T(-\bar{\psi}) = \frac{1}{i}\partial(-\bar{\psi}) = -\frac{1}{i}\bar{\partial\psi} = J\left(\frac{1}{i}\partial\psi\right) = JT\psi.$$

This way von Neumann's theorem can be used to prove existence of self-adjoint extensions of T .