SELF-ADJOINT EXTENSIONS

1. Introduction

We have seen that the issue of self-adjointness is subtle when dealing with unbounded operators.

Usually, we have at hand a differential operator which is manifestly symmetric on a convenient domain of regular functions, say in the Schwartz class or infinitely smooth with compact support.

As we have seen in earlier lectures such an operator is closable. However essentially self-adjointness is not necessarily given, sometimes false and even there might not be self-adjoint extensions at all.

The issue is of great matter in mathematical physics as if essential self-adjointness fails to hold, then the question arises to decide which one of the possible self-adjoint extension (if they exist at all) describes the considered system (in particular which one is to choose to generate the dynamics e^{-itH}).

In this part we give a framework to study the existence of self-adjoint extensions of a symmetric operator. We then illustrate the method with the simple example of $-i\frac{\mathrm{d}}{\mathrm{d}x}$ on $C_0^\infty(0,1)$ [1].

Remark 1. *Throughout this part A denotes a symmetric operator (densely defined) on a Hilbert space $\mathcal{H}$. Its domain is written* $\mathrm{dom}(A)$.

Furthermore the complex conjugation of a complex number z is written z^* so that the notation $\overline{(\cdot)}$ is kept for the closure of operators or of subset in $\mathcal{H}$.

The important (necesary and sufficient) condition to remember is the equality of the defect indices of A:

$$d_\pm := \dim \ker(A^* \mp i).$$

2. A criterion for essential self-adjointness

We start with a criterion for self-adjointness.

Lemma 2. *Let A sym. on $\mathcal{H}$. If there exists $z \in \mathbb{C}$ such that* $\mathrm{ran}(A+z) = \mathrm{ran}(A+z^*) = \mathcal{H}$, *then A is self-adjoint.*

Proof. Let $\psi \in \mathrm{dom}(A^*)$: let us show that $\psi \in \mathrm{dom}(A)$. By assumption there exists $\chi \in \mathrm{dom}(A)$ with $(A+z^*)\chi = (A^*+z^*)\psi$. For all $\varphi \in \mathrm{dom}(A)$ we thus have:

$$\begin{aligned}\langle \psi, (A+z)\varphi\rangle &\overset{def}{=} \langle A^*\psi + z^*\psi, \varphi\rangle,\\ &= \langle (A+z^*)\chi, \varphi\rangle,\\ &\overset{def}{=} \langle \chi, (A+z)\varphi\rangle.\end{aligned}$$

As $\mathrm{ran}(A+z) = \mathcal{H}$, we obtain $\psi = \chi \in \mathrm{dom}(A)$. □

[1] there is no need for this theory to study the s.a. extensions in this case, but it is always good to check one result on something we understand well.

The criterion for essential self-adjointness is the following.

Lemma 3. *A symmetric operator A is essentially s.a. if and only if there exists $z \in \mathbb{C} \setminus \mathbb{R}$ such that*

$$\overline{\operatorname{ran}(A-z)} = \overline{\operatorname{ran}(A-z^*)} = \mathcal{H},$$

or equivalently:

$$\ker(A^* - z) = \ker(A^* - z^*) = \{0\}.$$

Remark 4. *As $\mathbb{C} \setminus \mathbb{R} \subset \rho(A)$, if the condition holds for some $z \in \mathbb{C} \setminus \mathbb{R}$, it also holds for another $z_0 \in \mathbb{C} \setminus \mathbb{R}$ by the identity:*

$$(A - z_0)\psi = (A - z_0)(A - z)^{-1}(A - z)\psi, \;\; \psi \in \operatorname{dom}(A).$$

Indeed, as $(A - z_0)(A - z)^{-1} \in \mathcal{L}(\mathcal{H})$ is invertible, if $\operatorname{ran}(A - z)$ is dense, then so is $\operatorname{ran}(A - z_0)$.

Proof. *Claim:* We have the equalities

$$\overline{\operatorname{ran}(A-z)} = \operatorname{ran}(\overline{A} - z) \quad \& \quad \overline{\operatorname{ran}(A-z^*)} = \operatorname{ran}(\overline{A} - z^*).$$

Using the claim and Lemma 2, we get that $\overline{A}$ is s.a.

Let us show the claim. this follows from the auxiliary result:

Lemma 5 (Aux. res.)**.** *Let A sym. on $\mathcal{H}$. For $z \in \mathbb{C} \setminus \mathbb{R}$, $(A - z)$ is injective and its inverse $(A-z)^{-1} : \operatorname{ran}(A-z) \to \operatorname{dom}(A)$ is bounded with norm smaller than $|\operatorname{Im}(z)|^{-1}$.*

Proof of Aux. res. Let $\psi \in \operatorname{dom}(A)$ and $z = x + iy$ with $x, y \in \mathbb{R}$. As A is symmetric there holds:

$$\begin{aligned}\langle (A-z)\psi, (A-z)\psi\rangle &= \|A\psi\|_{\mathcal{H}}^2 + x^2\|\psi\|_{\mathcal{H}} - 2x\langle A\psi, \psi\rangle + y^2\|\psi\|_{\mathcal{H}}^2, \\ &\geq y^2\|\psi\|_{\mathcal{H}}^2.\end{aligned}$$

We have used the Cauchy-Schwarz inequality and $2ab \leq a^2 + b^2$. Hence $(A - z)$ is injective and its inverse $(A - z)^{-1} : \operatorname{ran}(A - z) \to \operatorname{dom}(A)$ is bounded with bound $|y|^{-1}$.

We consider the graph of $(A - z)^{-1}$:

$$\Gamma\,(A-z)^{-1} := \big\{((A-z)\psi, \psi), \;\; \psi \in \operatorname{dom}(A)\big\}.$$

Let us write $\varphi = (A - z)\psi$ for $\psi \in \operatorname{dom}(A)$: we have

$$\|\psi\|_{\mathcal{H}} \leq |y|^{-1}\|\varphi\|_{\mathcal{H}}. \tag{1}$$

By the above bound, the operator $(A-z)^{-1}$ can be extended to the closure of its domain $\operatorname{ran}(A - z)$ and:

$$\operatorname{dom}\left(\overline{(A-z)^{-1}}\right) = \overline{\operatorname{dom}(A-z)^{-1}}.$$

We check this claim by studying the closure of $\Gamma\,(A-z)^{-1}$. Let (φ_n) be a sequence of $\operatorname{dom}(A-z)^{-1}$ with $\varphi_n \to \varphi'$ and $\psi_n = (A-z)^{-1}\varphi_n \to \psi'$. By (1), we have $\|\psi_n\|_{\mathcal{H}} \leq |y|^{-1}\|\varphi_n\|_{\mathcal{H}}$, hence the closure of the graph is also a graph. This also shows the equality on the domains. This ends the proof if we notice that $\Gamma\,(A-z)^{-1}$ is, up to the switch $(\varphi, \psi) \mapsto (\psi, \varphi)$ the graph of $(A - z)$. Hence:

$$\overline{\operatorname{ran}(A-z)} = \overline{\operatorname{dom}(A-z)^{-1}} = \operatorname{dom}\left(\overline{(A-z)^{-1}}\right) = \operatorname{ran}\left(\overline{A} - z\right),$$

which ends the proof. □

3. Self-adjoint extensions

As said above we choose $z = i$ to simplify. The outcome is that a particular role is played by $\mathrm{ran}(A-i)$ and $\mathrm{ran}(A-i)$, or their orthogonal $\ker(A^*+i)$ and $\ker(A^* - i)$.

Definition 1. *For A sym. we call $K_\pm := \ker(A^* \mp i)$ the deficiency spaces and their dimension $d_\pm$ the defect indices.*

Furthermore $V := (A - i)(A + i)^{-1} : \mathrm{ran}(A + i) \to \mathrm{ran}(A - i)$ is called its Cayley transform.

Theorem 6. *The Cayley transform defines a bijection between the set of all symmetric operators A and the set of all libear isometric [2] operators V for which $(1 - V) : \mathrm{dom}(V) \to \mathrm{ran}(1 - V)$ has dense range and trivial kernel.*

Remark 7. *Above we will see that* $\mathrm{ran}(1 - V)$ *coincides with* $\mathrm{dom}(A)$ *and that we have*

$$A = i(1 + V)(1 - V)^{-1} \tag{2}$$

This theorem is proven below in Section 6

From Lemma 2, we get that a self-adjoint operator corresponds to that for which the Cayley transform is *unitary* (that is defined on the whole space $\mathcal{H}$). Assume that A admits a self-adjoint extension A_1. There holds $\mathrm{ran}(A_1 \pm i) = \mathcal{H}$ and we have:

$$\begin{aligned} \mathrm{ran}(A_1 \pm i) = \mathcal{H} &= \overline{\mathrm{ran}(A \pm i)} \overset{\perp}{\oplus} \ker(A^* \mp i), \\ &= \mathrm{ran}(\overline{A} \pm i) \overset{\perp}{\oplus} \ker(A^* \mp i). \end{aligned}$$

Let us consider the Cayley transforms V and V_1 of A and A_1 respectively. As $A \subset A_1$, then V_1 also extends V and as they are both isometric, then V_1 defines also an isometry between the two deficiency spaces. Thus a necessary condition for A to have a self-adjoint extension is that they must have the same dimension. From the remark, we get that an element $\psi \in \mathrm{dom}(A_1)$ can be decomposed as:

$$\psi = \psi_0 + (1 - V)\varphi_+,\ \psi_0 \in \mathrm{dom}(\overline{A}),\ \varphi_+ \in \ker(A^* - i), \tag{3}$$

and from (2) we have:

$$A_1\psi = \overline{A}\psi_0 + i(1 + V)\varphi_+.$$

Observe also that $V\varphi_+ = \varphi_- \in \ker(A^* + i)$.

Remark 8. *We can show in fact that the decomposition* (3) *is unique. If we introduce the graph norm w.r.t. A^*:*

$$\|\psi\|^2_{A^*} = \|\psi\|^2_{\mathcal{H}} + \|A^*\psi\|^2_{\mathcal{H}},\ \psi \in \mathrm{dom}(A^*),$$

with corresponding inner product

$$\langle\psi, \varphi\rangle_{A^*} := \langle\psi, \varphi\rangle + \langle A^*\psi, A^*\varphi\rangle,$$

[2] that is which conserves the norm $\|\cdot\|_{\mathcal{H}}$, or equivalently the inner product $\langle\cdot,\cdot\rangle$

then the following decomposition is orthogonal w.r.t. this inner product:

$$\mathrm{dom}(\overline{A}) \overset{\perp}{\oplus} \ker(A^* - i) \oplus \ker(A^* + i). \tag{4}$$

In particular the decomposition (3) *is orthogonal w.r.t. this inner product. This is left as an exercise.*

Conversely, if the defect indices are equal, it is *sufficient* to consider a linear isometric operator $U : \ker(A^* - i) \to \ker(A^* + i)$ to *define* a self-adjoint extension A_1 of A by setting:

$$\begin{cases} \mathrm{dom}(A_1) := \{\psi_0 + (\varphi_+ + U\varphi_+),\ \psi \in \mathrm{dom}(\overline{A}),\ \varphi_+ \in \ker(A^* - i)\}, \\ A_1(\psi_0 + (\varphi_+ + U\varphi_+)) := A^*(\psi_0 + (\varphi_+ + U\varphi_+)) = \overline{A}\psi_0 + i(\varphi_+ - U\varphi_+). \end{cases}$$

By construction it extends A, we can easily check that it is symmetric and closed (with the help of (4)). At last $\ker(A_1^* \mp i) = \{0\}$ for the following reason. Pick $\psi_\pm \in \ker(A_1^* \mp i) \subset \ker(A^* \mp i)$, we have:

$$0 = \langle \psi_+, (A_1 + i)(\psi_+ + U\psi_+)\rangle = \langle \psi_+, 2i\psi_+\rangle = 2i\|\psi_+\|_{\mathcal{H}}^2,$$
$$0 = \langle \psi_-, (A_1 - i)(U^{-1}\psi_- + \psi_-)\rangle = \langle \psi_-, -2i\psi_-\rangle = -2i\|\psi_-\|_{\mathcal{H}}^2,$$

which yields $\psi_+ = \psi_- = 0$. By Lemma (2) (with $z = i$), A_1 is self-adjoint.

We thus obtained the main result.

Theorem 9. *A symmetric operator A has s.a. extensions if and only if its defect indices are equal (may be both infinite). A s.a. extension $A \subset A_1$ has a Cayley transform $V_1 \in \mathcal{L}(\mathcal{H})$ which is unitary. Furthermore there holds:*

$$\mathrm{dom}(A_1) = \mathrm{ran}(1 - V_1) = \mathrm{dom}(\overline{A}) + (1 - V_1)\ker(A^* - i),$$

and for $\psi = \psi_0 + (1 - V_1)\varphi_+ \in \mathrm{dom}(A_1)$ we have

$$A_1(\psi + (1 - V_1)\varphi_+) = \overline{A}\psi + i(\varphi_+ + V_1\varphi_+).$$

4. Illustration of the method

We consider the operator $A := -i\frac{\mathrm{d}}{\mathrm{d}x}$ on $C_0^\infty(0,1)$, or, up to closing it, on $H_0^1(0,1)$. It is obviously symmetric on $\mathcal{H} = L^2(0,1)$, and it is a classical result that its self-adjoint extensions A_θ are given by:

$$\mathrm{dom}(A_\theta) := \{\psi \in H^1(0,1),\ \psi(0) = e^{i\theta}\psi(1)\}.$$

The s.a. extensions are prescribed by the transmission conditions across $1^- \to 0^+$ (think of $L^2(0,1)$ as $L^2(\mathbb{R}/\mathbb{Z})$).

We check this result with the method explained in the previous section.

1. Determination of A^*. Let $\psi \in \mathrm{dom}(A^*)$, by definition this means that there exists $\chi \in L^2(0,1)$ such that for all $\varphi \in \mathrm{dom}(A) = C_0^\infty(0,1)$ we have:

$$\langle \psi, A\varphi\rangle_{L^2} = \langle \chi, \varphi\rangle_{L^2}, \text{ that is } -i\langle \psi, \varphi'\rangle_{L^2} = \langle \chi, \varphi\rangle_{L^2}.$$

This is precisely the definition of $H^1(0,1)$, and $A^* = -i\frac{\mathrm{d}}{\mathrm{d}x}$ with $\mathrm{dom}(A^*) = H^1(0,1)$.

We recall that this space is embedded in the space of absolutely continuous functions, and that its elements admit a 1/2-Hölder representent. This simply follows from:

$$\begin{aligned}|\psi(x)-\psi(y)| &\le \int_x^y |\psi'(s)|\mathrm{d}s,\\ &\le \sqrt{\int_x^y \mathrm{d}s \int_x^y |\psi'(s)|^2\mathrm{d}s},\\ &\le \sqrt{|x-y|}\|\psi'\|_{L^2}.\end{aligned}$$

2. Determination of $\ker(A^*\mp i)$. Let $\psi\in\ker(A^*\mp i)$. This means that on $(0,1)$, it satisfies the O.D.E.

$$-i\psi'\mp i\psi=0 \text{ that is } \psi'=\mp\psi.$$

So $\psi(x)$ is colinear to e^{-x} resp. e^{x}. We normalize them and defines:

$$\varphi_+(x):=\sqrt{\frac{2}{1-e^{-2}}}e^{-x} \quad \& \quad \varphi_-(x):=\sqrt{\frac{2}{e^2-1}}e^{x}.$$

3. Discussion on the s.a. extensions. Thus the defect indices are $(1,1)$ and the s.a. extensions are parametrized by the unitary operator from $\ker(A^*-i)=\mathbb{C}\varphi_+\simeq\mathbb{C}$ to $\ker(A^*+i)=\mathbb{C}\varphi_-\simeq\mathbb{C}$. The latter set is topologically the circle $\mathbb{S}^1$ with corresponding unitaries:

$$U_z\lambda\varphi_+:=z\lambda\varphi_-,\ z=e^{i\tau}\in\mathbb{S}^1,\ \lambda\in\mathbb{C}.$$

The corresponding s.a. extensions are:

$$\begin{cases}\mathrm{dom}(A_z)=\big\{\psi_0+\lambda(\varphi_++z\varphi_-),\ \psi_0\in H_0^1(0,1),\ \lambda\in\mathbb{C}\big\},\\ A_z\big(\psi_0+\lambda(\varphi_++z\varphi_-)\big)=-i\psi_0'+i\lambda(\varphi_+-\varphi_-).\end{cases}$$

4. Link with the transmission condition. Let us check that there is a one-to-one correspondence between the complex number z and the the parameter in the transmission conditions. Let $\psi\in\mathrm{dom}(A_z)$ with $\psi=\psi_0+\lambda(\varphi_++z\varphi_-)$, with $\lambda\neq0$.

There holds $\psi(0)=\lambda(\varphi_+(0)+z\varphi_-(0))\neq0$ and $\psi(1)=\lambda(\varphi_+(1)+z\varphi_-(1))\neq0$, and:

$$\frac{\psi(0)}{\psi(1)}=\frac{\varphi_+(0)+z\varphi_-(0)}{\varphi_+(1)+z\varphi_-(1)}=\frac{e+z}{1+ez}=:\alpha_z.$$

It is straightforward to check $|\alpha_z|=1$, and conversely this relation can be inversed:

$$z=\frac{e-\alpha_z}{\alpha_z e-1}.$$

The case $z=1$, that is $\alpha=1$, corresponds to the well-known periodic boundary conditions, or equivalently to the extension with domain $H^1(\mathbb{R}/\mathbb{Z})$.

5. A criterion for the existsence of s.a. extensions

We give a criterion for the existence of s.a. extensions due to von Neumann.

Theorem 10. *Let A sym. on $\mathcal{H}$. Assume that there exists a conjugation C that maps* dom(A) *onto itself, that is that there exists an* antilinear *map $C.\mathcal{H} \to \mathcal{H}$ so that $C^2 = 1$. Assume firthermore that that $AC = CA$, then A has s.a. extensions.*

Proof. As $C\,\mathrm{dom}(A) \subset \mathrm{dom}(A)$, by applying C a second time, we get $\mathrm{dom}(A) \subset C\,\mathrm{dom}(A)$ and the equality of the two sets. Let $\varphi_+ \in \ker(A^* - i)$. For all $\psi \in \mathrm{dom}(A)$, there holds:

$$\begin{aligned} 0 = \langle \varphi_+, (A+i)\psi\rangle &= \overline{\langle C\varphi_+, C(A+i)\psi\rangle}, \\ &\overline{\langle C\varphi_+, (A-i)C\psi\rangle}, \end{aligned}$$

hence $C\ker(A^* - i) \subset \ker(A^* + i)$. By symmetry we have $C\ker(A^* + i) \subset \ker(A^* - i)$, and the two deficiency spaces are (anti)-isomorphic through C. □

6. Proof of Theorem 6

A **determines** V. We first check that V is a linear isometry.

Let $\psi \in \mathrm{dom}(A)$. As A is sym, there holds:

$$\begin{aligned} \|(A \pm i)\psi\|^2_{\mathcal{H}} &= \|A\psi\|^2_{\mathcal{H}} + \|\psi\|^2_{\mathcal{H}} + \pm i\big(\langle A\psi, \psi\rangle - \langle \psi, A\psi\rangle\big), \\ &= \|A\psi\|^2_{\mathcal{H}} + \|\psi\|^2_{\mathcal{H}}. \end{aligned}$$

Hence

$$V : (A+i)\psi \in \mathrm{ran}(A+i) \mapsto (A-i)\psi \in \mathrm{ran}(A-i).$$

is isometric.

A computation yields the following equality (to be read as maps from $\mathrm{dom}(V) \to \mathcal{H}$):

$$\begin{aligned} (1 \pm V) &= (A+i)(A+i)^{-1} \pm (A-i)(A+i)^{-1}, \\ &= \big[(A+i) \pm (A-i)\big](A+i)^{-1}, \\ &= \begin{cases} 2A(A+i)^{-1}, \\ 2i(A+i)^{-1}. \end{cases} \end{aligned}$$

In particular $\mathrm{ran}(1-V) = 2i(A+i)^{-1}\,\mathrm{ran}(A+i) = \mathrm{dom}(A)$ is dense. Furthermore we have:

$$A = i(1+V)(1-V)^{-1}. \tag{5}$$

At last we check that $\ker(1-V)$ is trivial, that is $\ker\big((A+i)^{-1}\big)_{|\mathrm{ran}(A+i)} = \{0\}$. Let $(A+i)\psi \in \mathrm{ran}(A+i)$. As shown above we have:

$$\|(A+i)\psi\|^2_{\mathcal{H}} = \|A\psi\|^2_{\mathcal{H}} + \|\psi\|^2_{\mathcal{H}},$$

hence if $\psi = 0$ then $(A+i)\psi = 0$.

V **determines** A. Conversely let $V : \mathrm{dom}(V) \to \mathcal{H}$ be a linear isometry. We use (5) as a definition of $A_V : \mathrm{ran}(1-V) \to \mathrm{ran}(1+V)$. By assumption it is both well and densely defined.

We check that A_V is a symmetric operator. As V is isometric, for $\psi \in \mathrm{dom}(V)$, we have:

$$\langle (1 \pm V)\psi, (1 \mp V)\psi \rangle = \pm 2i\mathrm{Im}\langle V\psi, \psi \rangle.$$

Hence for all $(1-V)\psi \in \mathrm{dom}(A_V)$, there holds:

$$\begin{aligned} \langle A_V\psi, \psi \rangle &\overset{\text{def}}{=} -i\langle (1+V)\psi, (1-V)\psi \rangle, \\ &= 2\mathrm{Im}\langle V\psi, \psi \rangle, \\ &= i\langle (1-V)\psi, (1+V)\psi \rangle, \\ &\overset{\text{def}}{=} \langle \psi, A_V\psi \rangle. \end{aligned}$$

At last, let us check that V is the Cayley transform of A_V. We have the following equality of operators defined from $\mathrm{dom}(A_V) = \mathrm{ran}(1-V)$ to $\mathcal{H}$.

$$\begin{aligned} (A_V \pm i) &= i(1+V)(1-V)^{-1}, \\ &= i\big[(1+V) \pm (1-V)\big](1-V)^{-1}, \\ &= \begin{cases} 2i(1-V)^{-1}, \\ 2iV(1-V)^{-1}. \end{cases} \end{aligned}$$

Tthis gives the following equality of operators defined from $\mathrm{ran}(A_V + i)$ to $\mathrm{ran}(A_V - i)$:

$$(A_V - i)(A_V + i)^{-1} = 2iV(1-V)^{-1}\big[2i(1-V)^{-1}\big]^{-1} = V.$$

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