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# SELF-ADJOINT EXTENSIONS FOR QUANTUM PHYSICS

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# Contents

**Abstract**: The main goal of this work is to provide techniques for finding self-adjoint extensions to unbounded operators, widely used in Quantum Physics. For that we use and study the Cayley method, concluding in the existance of a bijection between self-adjoint extensions and isometries between the deficiency subspaces of the Cayley transform. Using this knowledge we briefly parameterise the 1D, 2D and nD cases with possible self-adjoint extensions, and after introducing Sobolev spaces, we perform in more detail the search of self-adjoint extensions of the hamiltonian and laplacian operators.

**Abstract**: L'objectiu principal d'aquest treball és proporcionar tècniques per a trobar extensions autoadjuntes de operadors no afitats, àmpliament utilitzats en física quàntica. Per a això introduïm i desenvolupem el mètode de Cayley, i concloem en l'existència d'una bijecció entre extensions autoadjuntes i isometries entre els subespais de deficiència de la transformada de Cayley. Fem servir aquest coneixement per a parametritzar els casos 1D, 2D i nD on és possible trobar extensions autoadjuntes, i després d'introduïr els espais de Sobolev, duem a terme en més detall la cerca d'extensions autoadjuntes del hamiltonià i el laplacià.

# Chapter 1

# Introduction

## 1.1 Physical motivations

In Quantum Physics, particles (massive or not) and groups thereof are characterised by their *state* at a given space-time croordinate. Said state, also called its *wave function*, is a normalised element of a Hilbert space. The act of "measuring" a certain magnitude (energy, angular momentum module, third component of the spin, etc.) corresponds to applying an operator to the state - the hamiltonian for total energy, the spatial laplacian for squared momentum, etc. If applying an operator to a state results in the same state multiplied by an n-dimensional constant, then such a state is called an eigenstate of that operator, and the multuplicative constant or eigenvalue will be the value obtained whenever the operator's corresponding magnitude is measured.

If the state $\Psi$ of a particle isn't an eigenstate of the operator $T$, then that state can be expressed as a unique sum $\Psi = \sum_i a_i \Psi_i$, where $a_i \in \mathbb{C}$ and $\Psi_i$ are all eigenstates of $T$. Performing a measure of the magnitude associated to $T$ will then return one of any of the eigenvalues $\lambda_i$ at random, each one with a probability of $|a_i|^2$. Also, after performing the measure, the particle's state will change to become the eigenstate of that eigenvalue, the one randomly chosen one by reality. We say that the wave function *collapses* into an eigenstate upon being obvserved.

In Quantum Mechanics, obvservables must be self-adjoint operators in order for the concept of their *expected value* to make sense, but that is not the only reason for the interest in searching for self-adjoint extensions.

The hamiltonian operator $\mathscr{H}$ is very important not only because its eigenstate is the energy, but also because it gives the temporal evolution of a state, as can be clearly shown in the time-dependent Schrödinguer equation:

$$\mathscr{H}\Psi = i\frac{h}{2\pi}\frac{d}{dt}\Psi. \tag{1.1}$$

As we said, the states must always be normalised, $||\Psi|| = 1$, so that they can be seen as probability distributions regarding eigenvalues of observables. So we want their evolution in time to be unitary: For a transform $U(t) = e^{\mathscr{H}t}$ to be unitary, $1 = (\Psi(x,\ t),\ \Psi(x,\ t)) = (U(t)\Psi(x),\ U(t)\Psi(x))$, it has to be generated by operators $\mathscr{H}$ that are self-adjoint; hence why the hamiltonian is one of the particular operators we will treat explicitly on chapter 5, with the other being the laplacian $\bigtriangledown^2$, which in the non-relativistic case corresponds to the kinetic component of the hamiltonian:

$$i\frac{h}{2\pi}\frac{d}{dt}\Psi = (\frac{-h^2}{8\pi^2\mu}\bigtriangledown^2 + V)\Psi. \tag{1.2}$$

## 1.2 Structure of this work

We start by introducing the basic concepts and theorems of operator theory that we will use throughout this work, from Hermitan spaces and adjoints to symmetric and self-adjoint operators.

Then we introduce the Cayley transform of a self-adjoint operator and prove that it is unitary, explain the Cayley method for finding self-adjoint extensions by finding unitary extensions of the Cayley transform of a symmetrical operator and prove why it works, and parameterise the one-dimensional, two-dimensional, and n-dimensional cases where it is possible to find self-adjoint extensions.

In the next chapter we break away from self-adjoint extensions and instead introduce the concepts of weak derivative and Sobolev space, and enunciate the trace theorem, all of which we will make use in the following chapter.

Lastly, we apply our results of studying the Cayley method to finding self-adjoint extensions to the hamiltonian and the laplacian operators (without physical constants), differentiating the cases $H[0,\ 1]$ and $H[0,\ \infty)$ in both operators.

# Chapter 2

# Basics of operator theory

**Definition 2.1.** *Let $H$ be a Hilbert space with scalar or inner product $(\cdot,\ \cdot)$ and norm $||f|| = (f, f)^{1/2}\ \forall f \in H$. We define an* operator in $H$ *as a linear mapping $T$ with domain $\mathscr{D}(T) \subset H$ and range $\mathscr{R}(T) \subset H$, both subspaces.*

Unless it's stated otherwise, it is not assumed that $T$ is bounded (relative to the norm topology inherited from $H$).

**Definition 2.2.** *Given two topological vector spaces $X$ and $Y$, $\mathscr{B}(X, Y)$ will denote the vector space of bounded operators of $X$ into $Y$, with respect to the usual definitions of addition and multiplication by scalars. We'll abbreviate $\mathscr{B}(X, X)$ to $\mathscr{B}(X)$.*

**Definition 2.3.** *Let $T$ and $S$ be operators in $H$ such that $\mathscr{D}(T) \subset \mathscr{D}(S)$ and $Sx = Tx\ \forall x \in \mathscr{D}(T)$. $S$ is then called an* extension of $T$*, and we will mark so with the notation*

$$T \subset S. \tag{2.1}$$

**Definition 2.4.** *The* graph *of an operator $T$ in $H$ is the subspace $\mathscr{G}(T) \subset H \times H$ formed by the ordered pairs $\{x, Tx\}\ \forall x \in \mathscr{D}(T)$. Since $H$ is a Hilbert space with inner product $(\cdot,\ \cdot)$, we can make $H \times H$ into a Hilbert space by defining the inner product of two elements $\{a,\ b\}$ and $\{c,\ d\}$ of $H \times H$ as*

$$(\{a,\ b\},\ \{c,\ d\}) = (a,\ b) + (c,\ d). \tag{2.2}$$

It follows that $S$ is an extension of $T$ if and only if $\mathscr{G}(T) \subset \mathscr{G}(S)$.

**Definition 2.5.** *The* closure *of a set $M$, usually written as $\bar{M}$, is the smallest closed set that contains $M$.*

Obviously, the closure of a closed set is the same set.

**Definition 2.6.** *An operator $T$ in $H$ is* closed *when its graph is a closed subspace of $H \times H$.*

**Definition 2.7.** The *orthogonal complement* of a subspace $M \subset H$ is the subspace

$$M^{\perp} = \{y \in H \mid (x,\ y) = 0\ \forall x \in M\} \tag{2.3}$$

which is always closed due to the continuity of the inner product.

**Theorem 2.8.** *If $M$ is a closed subspace of $H$, then*

$$H = M \oplus M^{\perp}. \tag{2.4}$$

We will not demonstreate this theorem [1], but we will make use of some of its corollaries, each one immedieately derived from the previous one:

1. $M^{\perp} = \bar{M}^{\perp}$, where $\bar{M}$ is the closure of $M$.
2. If $M$ is closed, $M^{\perp\perp} = M$.
3. $M^{\perp\perp} = \bar{M}$

**Definition 2.9.** *When $T$ is injective, we can define its inverse $T^{-1}$ with $\mathscr{D}(T^{-1}) = \mathscr{R}(T)$ and $\mathscr{R}(T^{-1}) = \mathscr{D}(T)$ as $T^{-1}y = x$ when $Tx = y$.*

To proceed we need $T^*$, the adjoint to $T$, an operator such that $(Tx,\ y) = (x,\ T^*y)\ \forall x \in \mathscr{D}(T),\ y \in \mathscr{D}(T^*)$. Its domain will be constructed as

$$\mathscr{D}(T^*) = \{y \in H \mid x \to (Tx,\ y) \text{ is continuous on } \mathscr{D}(T)\} \tag{2.5}$$

with the condition that $\mathscr{D}(T)$ be dense for $T^*$ to be uniquely determined. The reason is that $\forall y \in H$ such that the linear functional $x \to (Tx,\ y)$ is continuous on $\mathscr{D}(T)$, by the Hahn-Banach theorem there exists an extension $F$ of said functional on $H$, and then by the Riesz representation theorem, $\exists z \in H$ such that $F(x) = (x,\ z)$, so when we're restricted again to $\mathscr{D}(T)$,

$$\exists z \in H \mid (Tx,\ y) = (x,\ z)\ \forall x \in \mathscr{D}(T). \tag{2.6}$$

Now it follows that $T^*$ is uniquely determined by $T^*y = z$ if and only if $\mathscr{D}(T)$ is dense.

From now on we will assume the existence of the adjoint of any operator we mention, and consequently all operators will be assumed densely defined except when unless stated otherwise.

From the definition of $\mathscr{D}(T^*)$ it is obvious that any extension $S$ of $T$ features an adjoint operator of which $T^*$ will be an extension - that is, $T \subset S \implies S^* \subset T^*$. Any bounded operator $T$ in $H$ can be extended first to the dense closure $\overline{\mathscr{D}(T)}$ of $\mathscr{D}(T)$ by continuity and then to $H$ by linearity, setting $\widetilde{T}f = 0$ for all element $f$ in the orthogonal complement $\mathscr{D}(T)^{\perp}$. The adjoint $\widetilde{T}^*$ of such an extension then has $H$ for domain, and since $\mathscr{D}(\widetilde{T}^*) \subset \mathscr{D}(T^*)$, then the adjoint of any bounded operator has the whole space for domain.

Since we are working with unbounded operators, we will need these natural definitions for the domains of sums and products:

$$\mathscr{D}(S+T) = \mathscr{D}(s) \cap \mathscr{D}(T) \tag{2.7}$$

$$\mathscr{D}(ST) = \{x \in \mathscr{D}(T) \mid Tx \in \mathscr{D}(S)\}. \tag{2.8}$$

**Theorem 2.10.** *Let $S$, $T$ and $ST$ be operators in $H$. Then*

$$T^*S^* \subset (ST)^* \tag{2.9}$$

*and if $S \in \mathscr{B}(H)$, it holds that*

$$T^*S^* = (ST)^*. \tag{2.10}$$

*Proof.* Assume $x \in \mathscr{D}(ST)$ and $y \in \mathscr{D}(T^*S^*)$. Then, since (2.8) implies $\mathscr{D}(ST) \subset \mathscr{D}(T)$,

$$(Tx,\ S^*y) = (x,\ T^*S^*y), \tag{2.11}$$

because $S^*y \in \mathscr{D}(T^*)$. And since $Tx \in \mathscr{D}(S)$ and $y \in \mathscr{D}(S^*)$,

$$(STx,\ y) = (Tx,\ S^*y) = (x,\ T^*S^*y). \tag{2.12}$$

This proves the inclusion.
Suppose now that $S \in \mathscr{B}(H)$ (and therefore $S^* \in \mathscr{B}(H)$ and $\mathscr{D}(S) = \mathscr{D}(S^*) = H$) and $y \in \mathscr{D}((ST)^*)$. Then, for every $x \in \mathscr{D}(ST)$,

$$(Tx,\ S^*y) = (STx,\ y) = (x,\ (ST)^*y). \tag{2.13}$$

Therefore $S^*y \in \mathscr{D}(T^*)$ and so $y \in \mathscr{D}(T^*S^*)$. This proves the equality in the case $S \in \mathscr{B}(H)$. □

**Definition 2.11.** An operator $T$ in $H$ is *symmetric* if

$$(Tx,\ y) = (x,\ Ty)\ \forall x,\ y \in \mathscr{D}(T). \tag{2.14}$$

If $T$ is densely defined, then $T$ being symmetric is equivalent to

$$T \subset T^*. \tag{2.15}$$

**Definition 2.12.** $T$ is *self-adjoint* when $T = T^*$.

Note in particular that self-adjointness implies symmetry, and that when $T \in \mathscr{B}(H)$, the two coincide, but in general symmetry does not imply self-adjointness, as we will see in chapter 3.

For the next section, we will call $V$ the operator $V\{a,\ b\} = \{-b,\ a\}$ with domain $\mathscr{D}(V) = H \times H$.

**Theorem 2.13.** *If $T$ is an operator in $H$, then*

$$\mathscr{G}(T^*) = (V\mathscr{G}(T))^{\perp}. \tag{2.16}$$

*Proof.* Note that any element of $(V\mathscr{G}(T))^{\perp}$ can be written as $\{-Tx,\ x\}$ for some $x \in \mathscr{D}(T)$. Then the following equivalences prove that $\mathscr{G}(T^*) \subset [V\mathscr{G}(T)]^{\perp}$ if read from left to right, and $\mathscr{G}(T^*) \supset (V\mathscr{G}(T))^{\perp}$ if read from right to left:

$$\begin{aligned}\{y,\ z\} \in \mathscr{G}(T^*) \iff z = T^*y \iff \forall x \in \mathscr{D}(T),\ (V\{x,\ Tx\},\ \{y,\ z\}) = \\ = (\{-Tx,\ x\},\ \{y,\ T^*y\}) = -(Tx,\ y) + (x, T^*y) = 0 \iff \{y,\ z\} \in [V\mathscr{G}(T)]^{\perp}.\end{aligned} \tag{2.17}$$

□

**Corollary 2.14.** *If $T$ is an operator in $H$, then* $\operatorname{Ker} T^* = \mathscr{R}(T)^{\perp}$-

*Proof.* Considering that $y \in \text{Ker}(T^*) \iff T^*x = 0$, then it follows easily from the main theorem:

$$x \in \text{Ker}(T^*) \iff \{x,\ 0\} \in \mathscr{G}(T^*) \iff \{x,\ 0\} \in [V\mathscr{G}(T)]^{\perp} \iff x \in \mathscr{R}(T)^{\perp}. \quad (2.18)$$

□

**Theorem 2.15.** *If $T$ is an operator in $H$, then $T^*$ is closed.*

*Proof.* As said in Theorem 2.7, orthogonal complements of subspaces are closed, and so $\mathscr{G}(T^*) = (V\mathscr{G}(T))^{\perp}$ is closed in $H \times H$, making $T^*$ a closed operator in $H$. □

**Theorem 2.16.** *If $T$ is a closed operator in $H$, then $\mathscr{D}(T^*)$ is dense and $T^{**} = T$.*

*Proof.* Since $V$ is unitary (that is, both bijective and isometric) and $V^2 = -I$, then by Theorems 2.8 and 2.13,

$$(V\mathscr{G}(T^*))^{\perp} = (V(V\mathscr{G}(T))^{\perp})^{\perp} = \mathscr{G}(T)^{\perp\perp} = \mathscr{G}(T) \Rightarrow \mathscr{G}(T) \oplus V\mathscr{G}(T^*) = H \times H \quad (2.19)$$

where we've used the fact that $T$ being closed implies $(\mathscr{G}(T))^{\perp\perp} = \mathscr{G}(T)$. Let $z \in [\mathscr{D}(T^*)]^{\perp}$. Then

$$(\{0,\ z\},\ \{-T^*y,\ y\}) = 0\ \forall y \in \mathscr{D}(T^*), \quad (2.20)$$

and so $\{0,\ z\} \in [V\mathscr{G}(T^*)]^{\perp} = \mathscr{G}(T)$. This in turn means that $z = T(0) = 0$, making $\mathscr{D}(T^*)$ dense in $H$. Thus, $T^{**}$ can be defined, and we can use the equivalence

$$\mathscr{G}(T^{**}) = (V\mathscr{G}(T^*))^{\perp} = \mathscr{G}(T) \quad (2.21)$$

to show that $T^{**} = T$. □

Using this result alongside Theorem 2.15, we can deduce the following:

**Lemma 2.17.** *If $S$ is a symmetric operator in $H$, then $S$ is closable and its closure is $S^{**}$, which also is symmetric.*

*Proof.* The previous result guarantees that $S^{**}$ exists and is closed. Since $T^*$ is closed, then $S^{***} = (S^*)^{**} = S^*$. Remembering that $A \subset B \Rightarrow A^* \supset B^*$, and that $S$ being symmetric is equivalent to $S \subset S^*$, then $S \subset S^* \Rightarrow S^* \supset S^{**} \Rightarrow S^{**} \subset S^{***}$, and so $S^{**}$ is symmetric. And since $S^{**} = (S^*)^*$ means that $\mathscr{D}(S) \in \mathscr{D}(S^{**})$, we have $S \subset S^{**}$. In short, $S^{**}$ is a symmetric extension of $S$. And since given any other closed extension $T \supset S$, it would follow that $T^* \subset S^*$, and $T^{**} \supset S^{**}$, and with $T$ being closed, $T^{**} = T \supset S^{**}$ confirms that $S^{**}$ is the closure of $S$. □

# Chapter 3

# Self-Adjoint Extensions

An asymmetric operator $T$ such that $(Tx, y) \neq (x, Ty)$ for some $x,\ y \in \mathscr{D}(T)$ cannot be extended into a symmetric operator, for if $T \subset \hat{T}$ then $x,\ y \in \mathscr{D}(\widetilde{T})$ and $(\widetilde{T}x, y) = (Tx, y) \neq (x, Ty) \neq (x, \widetilde{T}y)$. Since our main objective is to obtain self-adjoint (and therefore symmetric) extensions, we will work mostly with symmetric operators as bases. From now on, unless we explicity say otherwise, any operator denoted as $A$ will be assumed to be self-adjoint, and any operator denoted as $S$ will be assumed to be symmetric and closed (since we can extend any symmetric operator $S$ into its closure $S^{**}$).

## 3.1 Cayley Transforms

### 3.1.1 Self-adjoint operators

Given a self-adjoint operator $A$ in $H$, we want to study the two mutually adjoint transforms

$$(A \mp iI)^{-1} \tag{3.1}$$

and prove that they are defined everywhere in $H$. This can also be seen by showing how the norms of their inverses,

$$||(A \mp iI)||^2 = (Af,\ Af) \mp i(f,\ Af) \pm i(Af,\ f) + (f,\ f) = ||Af||^2 + ||f||^2, \tag{3.2}$$

are zero if and only if $f = 0$, proving the existence of $(A \mp iI)^{-1}$ as inverses. This also means that

$$||(A \mp iI)f|| \geq ||f||, \quad ||(A \mp iI)^{-1}g|| \leq ||g|| \tag{3.3}$$

which shows that $(A \mp iI)^{-1}$ is continuous, which means that they are closed if coupled with $A$ and $(A \mp iI)$ being closed.

That $(A \mp iI)^{-1}$ are defined everywhere in $H$ is a consequence of them being both closed and everywhere dense in $H$. The latter can be proven by reasoning that, if they were not, then Theorem 2.8 would imply the existence of an element $h \neq 0$, $h \in \mathscr{D}((A \mp iI)^{-1})^{\perp} = \mathscr{R}(A \mp iI)^{\perp}$. But from

$$((A \mp iI)f,\ h) = 0 \tag{3.4}$$

it follows that $h \in \mathscr{D}((A \mp iI)^*) = \mathscr{D}(A \pm iI) = \mathscr{D}(A \mp iI)$, which Theorem 2.8 implies only happens for $h = 0$, contrary to our previous assumption. Therefore, $\mathscr{D}((A \mp iI)^{-1}) = H$. Note how on this last step we relied on the self-adjointness of $A$ by using the equivalence $\mathscr{D}((A \mp iI)^*) = \mathscr{D}(A \pm iI)$, as it will be important when we work with non-self-adjoint operators. Now we define $V$, the *Cayley transform of $A$*, as

$$V = (A - iI)(A + iI)^{-1}. \tag{3.5}$$

Since we have shown in (3.2) that $||(A + iI)f|| = ||(A - iI)f||$, we can develop

$$||Vf|| = ||(A - iI)(A + iI)^{-1}f|| = ||(A + iI)(A + iI)^{-1}f|| = ||f|| \tag{3.6}$$

to prove that the Cayley transform of self-adjoint operators is isometric. Since $\mathscr{D}(A - iI) = \mathscr{D}(A + iI) = \mathscr{R}((A + iI)^{-1})$, then $\mathscr{D}(V) = \mathscr{D}((A + iI)^{-1}) = H$, and $\mathscr{R}(V) = \mathscr{R}(A - iI) = H$. In other words, $V$ is bijective, which together with its isometry makes $V$ unitary by definition.

A final step of our incoming extending method will be recovering $A$ from $V$. If we define $f = (A + iI)^{-1}g$, then

$$(I + V)g = 2Af, \quad (I - V)g = 2if, \tag{3.7}$$

where we can see that $(I - V)g = 0 \iff f = 0$. Coupled with (3.2) implying that $f = 0 \iff g = 0$, we have proved the existence of $(I - V)^{-1}$, and so we can use the following recovery transform:

$$A = i(I + V)(I - V)^{-1}. \tag{3.8}$$

Let us compile our results:

**Lemma 3.1.** *Let $A$ be a self-adjoint operator in $H$. Then its Cayley transform, defined as*

$$V = (A - iI)(A + iI)^{-1} \tag{3.9}$$

*is a unitary operator in $H$, that is, $V \in \mathscr{B}(H)$ and $VV* = V^*V = I$; and $A$ can be recoverd from $V$ through the transform*

$$A = i(I + V)(I - V)^{-1}. \tag{3.10}$$

### 3.1.2 Symmetric operators

We have shown the properties of the Cayley transform of self-adjoint operators. Since our goal is to extend a symmetric operator $S$ into a self-adjoint one $A \supset S$, our general idea will be to obtain the Cayley transform $V$ of $S$ and extend it into another operator $\widetilde{V}$ that shows the properties of the Cayley transform of a self-adjoint operator, and then recover the self-adjoint extension $A$ of $S$ from $\widetilde{V}$ via (3.8).

Like before, we start by defining the Cayley transform, this time of $S$:

**Lemma 3.2.** *Let $S$ be a symmetric operator in $H$. Then its Cayley transform, defined as*

$$V = (S - iI)(S + iI)^{-1} \tag{3.11}$$

*is an isometric operator in $H$, and $S$ can be recoverd from $V$ through the transform*

$$S = i(I + V)(I - V)^{-1}. \tag{3.12}$$

We can use the equivalents of (3.2) and (3.6) to show that $V$ is still isometric, but we can't affirm that $V$ is unitary, since this time we can't guarantee that $V$ is bijective (and an unitary operator is one which is both bijective and isometric). Remember that for self-adjoint operators, we had to prove that $\mathscr{D}(V) = \mathscr{D}((A + iI)^{-1}) = H$ and $\mathscr{R}(V) = \mathscr{R}(A - iI) = H$, for which we used the property $\mathscr{D}((A - iI)^*) = \mathscr{D}(A + iI)$. However, the equivalent statement $\mathscr{D}((S - iI)^*) = \mathscr{D}(S + iI)$ is not necessarily true. We already know that a self-adjoint operator produces only a unitary Cayley transform $V$; now we will go a step further and prove that a unitary Cayley transform $V$ can only be produced by a self-adjoint initial operator.

Let us assume that the Cayley transform $V$ of $S$ is unitary, and let $g \in \mathscr{D}(S^*)$ and $g^* = S^*g$. Then

$$(Sf,\ g) = (f,\ g^*)\ \forall f \in \mathscr{D}(S), \tag{3.13}$$

and since $\mathscr{D}(S) = \mathscr{R}(I - V)$ as can be seen in (3.8) assures us we can express $f$ as $f = (I - V)h$, we have

$$(i(I + V)h,\ g) = ((i - V)h,\ g^*). \tag{3.14}$$

Separating the products, we can write

$$i(h,\ g) + i(Vh,\ g) = (h,\ g^*) - (Vh,\ g^*) \tag{3.15}$$

and use $V$'s unitary property $(Vx,\ Vy) = (x,\ y)$ to replace $(h,\ g)$ and $(h,\ g^*)$, rejoin the products, and obtain

$$(Vh,\ -iVg - ig - Vg^* + g^*) = 0. \tag{3.16}$$

Since $V$ being unitary means the above holds true for all $h \in H$, it follows that

$$-iVg - ig - Vg^* + g^* = 0 \tag{3.17}$$

which can be rearranged into certain expressions for $g$ and $g^*$:

$$g = (I - V)\frac{g - ig^*}{2}, \quad g^* = i(I + V)\frac{g - ig^*}{2}. \tag{3.18}$$

This expression of $g$, when compared to that of $S$ in (3.12), implies that $g \in \mathscr{D}(S)$ and $Sg = g^*$, both for all $g \in \mathscr{D}(S^*)$, and so $S^* = S$, and so $S$ is self-adjoint.

We have just seen then that a symmetric operator is self-adjoint if, and only if, its Cayley transform's domain is $\mathscr{D}(V) = H$. And since $V$ is also isometric regardless of self-adjointness, that amounts to being unitary. So if we make can extend $V$ into a unitary operator $\widetilde{V}$ by extending its domain to and range $H$, then upon applying (3.12) we will obtain a self-adjoint extension of $S$.

**Theorem 3.3.** *Let $S$ be a symmetric operator in $H$. Then the Cayley transform of $S$ will be unitary if, and only if, $S$ is self-adjoint.*

We can indicate $V$'s capacity for being or extending into a unitary operator, and therefore of $S$ to being or exteniding into a self-adjoint operator, with the help of the following two subspaces:

**Definition 3.4.** *Let $V$ be the Cayley transform of a symmetric operator $S$. Then the subspaces*

$$D_{+} = \mathscr{D}(V)^{\perp}, \quad D_{-} = \mathscr{R}(V)^{\perp} \tag{3.19}$$

*are called the* deficiency subspaces *of $S$ (or of its Cayley transform $V$), and their dimensions $d_{\pm} = \dim D_{\pm}$ the* deficiency indices*.*

Note that $D_{\pm} = \mathscr{R}(S \pm iI)^{\perp}$, easy to see just from looking at (3.12), and therefore $D_{\pm} = \operatorname{Ker}(S^{*} \mp iI)$. Since $S$ is closed, so is $V$, meaning that both $\mathscr{D}(V)$ and $\mathscr{R}(V)$ are closed, and so each one completes the space $H$ if summed with their orthogonal complements, the deficiency spaces. $V$ being unitary implies $\mathscr{D}(V) = \mathscr{R}(V) = H$ and so $D_{\pm} = \{0\}$, which in turn implies $d_{\pm} = 0$. Also, $d_{+} = d_{-} = 0$ implies $\mathscr{D}(V) = \mathscr{R}(V) = H$, which we proved suffices to imply $V$ is unitary. This coimplication is a most important result:

**Theorem 3.5.** *A closed symmetric operator $S$ is also self-adjoint if, and only if, its deficiency indices are both zero.*

The deficiency indices contain information about the possibilities of extending V. If $\widetilde{S} \supset S$ is symmetric and closed, its Cayley transform $V$ will be an extension of $V$, since $\mathscr{D}(\widetilde{V}) = \mathscr{R}(\widetilde{S} + iI) \supset \mathscr{R}(S + iI) = \mathscr{D}(V)$, and $\widetilde{V}$ being defined as (3.12) in terms of $\widetilde{S}$ instead of $S$ means that $\widetilde{V}x = Vx \ \forall x \in \mathscr{D}(V)$, ergo $\widetilde{V} \supset V$. The reciprocal is also true: Let $\widetilde{V}$ be an isometric extension of $V$. To show that $(I - \widetilde{V})^{-1}$ exists, consider that, if $(I - \widetilde{V})f = 0$, then $\forall g \in \mathscr{D}(I - \widetilde{V})$,

$$(f,\ (I - \widetilde{V})g) = (f,\ g) - (f,\ \widetilde{V}g) = (\widetilde{V}f,\ \widetilde{V}g) - (f,\ \widetilde{V}g) = ((I - \widetilde{V})f,\ \widetilde{V}g) = 0, \tag{3.20}$$

which means that $f \in \mathscr{R}(I - \widetilde{V})^{\perp} \subset \mathscr{R}(I - V)^{\perp} = \mathscr{D}(S)^{\perp}$, and since $\mathscr{D}(S)$ is dense in $H$, then $(I - \widetilde{V})f = 0 \iff f = 0$, proving the existence of $(I - \widetilde{V})^{-1}$. Now we can obtain the operator

$$\widetilde{S} = i(I + \widetilde{V})(I - \widetilde{V})^{-1} \tag{3.21}$$

which is obviously an extension of $S$, with $\mathscr{D}(\widetilde{S}) = \mathscr{R}(I - \widetilde{V}) \supset \mathscr{R}(I - V) = \mathscr{D}(S)$, and is symmetric: if $f',\ g' \in \mathscr{D}(\widetilde{S})$, then $f' = (I - \widetilde{V})f$ and $g' = (I - \widetilde{V})g$ for some $f,\ g \in H$, and

$$\begin{aligned} (\widetilde{S}f',\ g') &= (i(I + \widetilde{V})f,\ (I - \widetilde{V})g) = i[(\widetilde{V}f,\ g) - (f,\ \widetilde{V}g)] = \\ &= ((I - \widetilde{V})f,\ i(I - \widetilde{V})g) = (f',\ \widetilde{S}g'). \end{aligned} \tag{3.22}$$

When $V$ is extended into $\widetilde{V}$, and so is $S$ into $\widetilde{S}$, and we define $\hat{S}$ as the restriction of $\widetilde{S}$ in $\mathscr{D}(\hat{S}) = \mathscr{D}(\widetilde{S}) - \mathscr{D}(S)$, then the deficiency subspaces are also extended as $D_{\pm}(\widetilde{V}) = \mathscr{R}(\widetilde{S} \pm iI) = \mathscr{R}(S \pm iI) \oplus \mathscr{R}(\hat{S} \pm iI)$. Since both deficiency subspaces are extended in the same number of dimensions ($\dim(\mathscr{R}(\hat{S} + iI)) = \dim(\mathscr{R}(\hat{S} - iI))$), then $d_{+}$ and $d_{-}$ both decrease by the same number. This finally gives us a criteria to tell if a symmetric closed operator can be extended into a self-adjoint one:

**Theorem 3.6.** *A closed symmetric operator S has self-adjoint extionsion(s) if, and only if, its two deficiency indices are equal to one another.*

Furthermore, extending $V$ into an unitary operator $\widetilde{V}$ is equivalent to defining a bijective isometry $V_D$ from $D_+$ to $D_-$ and setting $\widetilde{V}(x) = V_D(x)\ \forall x \in D_+$.

**Theorem 3.7.** *There is a bijection between the self-adjoint extensions of S and the bijective isometries between $D_+$ and $D_-$.*

Now let us try the Cayley method.

## 3.2 Deficiency indices: cases $d_+ = d_-$

### 3.2.1 Linear bijective isometries

Before starting on breaking down, it will be useful to know how the linear bijective isometries between $D_+$ and $D_-$ will be parameterized. Note that, were $D_+$ and $D_-$ the same space, we would call such an isometry a unitary transformation - that is why it must be pameterized by unitary matrices.

**Theorem 3.8.** *Given subspaces $D_+$ and $D_-$, both of dimension n, and respective orthonormal bases $\{\phi_+^j\}_{j=1}^n$ and $\{\phi_-^j\}_{j=1}^n$ of them, then there is a bijection $U \to V_U$ between the set of $n \times n$ unitary matrices $\mathbb{U}(n) = \{U \in \mathbb{M}(n,\ \mathbb{C}) \mid UU^* = U^*U = I\}$ and the bijective isometries $V_U$ between $D_+$ and $D_-$, and these are*

$$\begin{array}{rcl} V_U:\ D_+ & \to & D_- \\ \vec{\phi}_+\vec{k}^\top & \to & \vec{\phi}_- U\vec{k}^\top \end{array} \tag{3.23}$$

*where $\vec{\phi}_\pm = \begin{pmatrix}\phi_\pm^1 & \dots & \phi_\pm^n\end{pmatrix}$ and $\vec{k}^\top \in \mathbb{C}^n$ is a vertical vector of complex coefficients akin to the coordinates of $\vec{\phi}_+\vec{k}^\top$ in base $\{\phi_+^j\}_{j=1}^n$.*

### 3.2.2 Case $d_\pm = 1$

Assume an operator $S$ with both deficiency indices equal to one.This means that both deficiency subspaces, $D_+$ and $D_-$, have dimension one. Let then $\{\phi_+\}$ and $\{\phi_-\}$ be normalised bases of $D_+$ and $D_-$, respectively, and so also generators of them (which is written as $D_\pm = \langle\phi_\pm\rangle$) with $||\phi_\pm|| = 1$, so that any element of $D_\pm$ can be written as $c\phi_\pm$, where $c \in \mathbb{C}$. Then any isometry $V_\theta$ from $D_+$ to $D_-$ takes the form

$$\begin{array}{rcl} V_\theta:\ D_+ & \to & D_- \\ c\phi_+ & \to & e^{i\theta}c\phi_- \end{array} \tag{3.24}$$

where $\theta \in [0, 2\pi)$. Note that, while we make use of $V$, we don't need to definte it explicitely - besides its definition based on $S$, we will see how it is enough to conisder it as

$$\begin{aligned} V: \mathscr{R}(S+iI) &\rightarrow \mathscr{R}(S-iI) \\ \phi_0 &\rightarrow V\phi_0. \end{aligned} \tag{3.25}$$

Now let us form $\widetilde{V}$, the unitary extension of $V$ via $V_\theta$:

$$\begin{aligned} \widetilde{V}: \mathscr{R}(S+iI)\oplus D_+ &\rightarrow \mathscr{R}(S-iI)\oplus D_- \\ \phi_0 + c\phi_+ &\rightarrow V\phi_0 + e^{i\theta}c\phi_-. \end{aligned} \tag{3.26}$$

As to constructing $A$ from $\widetilde{V}$, we consider that, since $\mathscr{D}(V)\oplus D_+ = H$, then $\forall\phi\in H\ \exists\phi_0\in\mathscr{D}(V),\ c\in\mathbb{C}$ such that $\phi=\phi_0+c\phi_+$, so we can develop $(I-\widetilde{V})\phi$ as

$$(I-\widetilde{V})(\phi_0+c\phi_+) = \phi_0 + c\phi_+ - V\phi_0 - ce^{i\theta}\phi_- = (I-V)\phi_0 + c(\phi_+ - e^{i\theta}\phi_-) \tag{3.27}$$

where, since $i(I+V)\phi_0 = S(I-V)\phi_0$, we can conclude that $(I-V)\phi_0\in\mathscr{D}(S)$. Now we can use the formula for the recovery of the self-adjoint extension $A$,

$$A = i(I+\widetilde{V})(I-\widetilde{V})^{-1} \tag{3.28}$$

and apply it to $(I-\widetilde{V})\phi$ to see how it behaves:

$$A(I-\widetilde{V})\phi = i(i+\widetilde{V})(\phi_0+c\phi_+) = i(I+V)\phi_0 + ic(\phi_+ + e^{i\theta}\phi_-). \tag{3.29}$$

We can simplify things further if we define $(I-V)\phi_0 = g\in\mathscr{D}(S)$ and consequently $i(I+V)\phi_0 = Sg$:

$$A(g + c(\phi_+ - e^{i\theta}\phi_-)) = Sg + ic(\phi_+ + e^{i\theta}\phi_-) \tag{3.30}$$

which shows that $A$ is an extension of $S$, with domain $\mathscr{D}(A) = \mathscr{D}(S)\oplus\langle\phi_+ - e^{i\theta}\phi_-\rangle$.

**Lemma 3.9.** *Let $S$ be a symmetric operator in $H$ with deficiency indices $d_\pm = 1$, and let $\{\phi_+\}$ and $\{\phi_-\}$ be normalised bases of $D_+$ and $D_-$, respectively. Then the self-adjoint extensions of $S$, $A_\theta \supset S$, can be parametrised by $\theta\in[0,\ 2\pi)$ in the form*

$$\begin{aligned} A:\theta:\ \mathscr{D}(S)\oplus\langle\phi_+ - e^{i\theta}\phi_-\rangle &\rightarrow \mathscr{R}(S)\oplus\langle\phi_+ + e^{i\theta}\phi_-\rangle \\ f + c(\phi_+ - e^{i\theta}\phi_-) &\rightarrow Sf + ic(\phi_+ + e^{i\theta}\phi_-)\ \forall f\in\mathscr{D}(S),\ c\in\mathbb{C}. \end{aligned} \tag{3.31}$$

### 3.2.3 Case $d_\pm = 2$

Just like before, we choose orthonormal bases $\{\phi_+^1,\ \phi_+^2\}$ and $\{\phi_-^1,\ \phi_-^2\}$ for $D_+$ and $D_-$. Now we must choose a *linear and bijective* isometry between $D_+$ and $D_-$, which means it must take the form of

$$\begin{aligned} V_U:\ D_+ &\rightarrow D_- \\ a\phi_+^1 + b\phi_+^2 &\rightarrow \vec{\phi_-}U\begin{pmatrix} a \\ b \end{pmatrix} \end{aligned} \tag{3.32}$$

where $\vec{\phi_-}$ is the $2\times 1$ matrix $\begin{pmatrix}\phi_-^1 & \phi_-^2\end{pmatrix}$ and $U$ is a unitary $2\times 2$ matrix, that is, a matrix of the form

$$U = e^{i\gamma}\begin{pmatrix} e^{i\alpha}\cos\theta & e^{i\beta}\sin\theta \\ -e^{-i\beta}\sin\theta & e^{-i\alpha}\cos\theta \end{pmatrix} \tag{3.33}$$

where $\alpha, \beta, \gamma, \theta \in [0,\ 2\pi)$. This means that $V_U$ depends on four real parameters, and consequently so does $\widetilde{V}$. From then we proceed analogously to the one-dimensional case, and end up with

$$A(g + (\vec{\phi_+} - \vec{\phi_-}U)\begin{pmatrix}a\\b\end{pmatrix}) = Sg + (\vec{\phi_+} + \vec{\phi_-}U)\begin{pmatrix}a\\b\end{pmatrix})\ \forall g \in \mathscr{D}(S) \tag{3.34}$$

which has been extended from $S$ to

$$\begin{aligned} \mathscr{D}(A) &= \mathscr{D}(S) \oplus \langle \phi_+^1 - \vec{\phi_-}U\begin{pmatrix}1\\0\end{pmatrix},\ \phi_+^2 - \vec{\phi_-}U\begin{pmatrix}0\\1\end{pmatrix}\rangle \\ \mathscr{R}(A) &= \mathscr{R}(S) \oplus \langle \phi_+^1 + \vec{\phi_-}U\begin{pmatrix}1\\0\end{pmatrix},\ \phi_+^2 + \vec{\phi_-}U\begin{pmatrix}0\\1\end{pmatrix}\rangle. \end{aligned} \tag{3.35}$$

**Lemma 3.10.** *Let $S$ be a symmetric operator in $H$ with deficiency indices $d_\pm = 2$, and let $\{\phi_+^1,\ \phi_+^2\}$ and $\{\phi_-^1,\ \phi_-^2\}$ be orthonormal basees of $D_+$ and $D_-$, respectively. Then the self-adjoint extensions of $S$, $A_U \ni S$, can be parameterised by the $2\times 2$ unitary matrices $U \in \mathbb{U}(2)$ in the form*

$$\begin{aligned} A : \mathscr{D}(S) \oplus \langle \phi_+^1 - \vec{\phi_-}U\begin{pmatrix}1\\0\end{pmatrix},\ \phi_+^2 - \vec{\phi_-}U\begin{pmatrix}0\\1\end{pmatrix}\rangle &\to \\ \to \mathscr{R}(S) \oplus \langle \phi_+^1 + \vec{\phi_-}U\begin{pmatrix}1\\0\end{pmatrix},\ \phi_+^2 + \vec{\phi_-}U\begin{pmatrix}0\\1\end{pmatrix}\rangle & \\ f + (\vec{\phi_+} - \vec{\phi_-}U)\begin{pmatrix}a\\b\end{pmatrix}) \to Sf + (\vec{\phi_+} + \vec{\phi_-}U)\begin{pmatrix}a\\b\end{pmatrix})\ \forall f \in \mathscr{D}(S),\ a, b \in \mathbb{C}. & \end{aligned} \tag{3.36}$$

### 3.2.4 General case $d_\pm = n$

As we can easily induce from the bidimensional case, given orthonormal bases $\{\phi_\pm^j \mid j \in \{1,\ ...,\ n\}\}$, we choose a unitary $n\times n$ matrix $U$ to define the isometry

$$\begin{aligned} V_U :\ D_+ &\to D_- \\ \vec{\phi_+}\vec{k}^\top &\to \vec{\phi_-}U\vec{k}^\top \end{aligned} \tag{3.37}$$

where $\vec{k}^\top$ is a complex $1\times n$ vector akin to the coordinates in base $\{\phi_+^j\}$ of the element of $D_+$ in question. Then the self-adjoint extension $A$ will be

$$A(g + (\vec{\phi_+} - \vec{\phi_-}U)\vec{k}^\top) = Sg + (\vec{\phi_+} + \vec{\phi_-}U)\vec{k}^\top\ \forall g \in \mathscr{D}(S) \tag{3.38}$$

and the extended domain and range will be

$$\begin{aligned} \mathscr{D}(A) &= \mathscr{D}(S) \oplus_{j=1}^n \langle (\phi_+ - \vec{\phi_-}U)\hat{e}_j^\top \rangle \\ \mathscr{R}(A) &= \mathscr{R}(S) \oplus_{j=1}^n \langle (\phi_+ + \vec{\phi_-}U)\hat{e}_j^\top \rangle \end{aligned} \tag{3.39}$$

where $\hat{e}_j^\top = (0, \ldots, 0, \overset{(j)}{1}, 0 \ldots, 0)^\top$.

**Lemma 3.11.** *Let $S$ be a symmetric operator in $H$ with deficiency indices $d_\pm = n$, and let $\{\phi_+^j\}_{j=1}^n$ and $\{\phi_-^j\}_{j=1}^n$ be orthonormal basees of $D_+$ and $D_-$, respectively. Then the self-adjoint extensions of $S$, $A_U \ni S$, can be parameterised by the $n \times n$ unitary matrices $U \in \mathbb{U}(n)$ in the form*

$$\begin{array}{rcl} A: \mathscr{D}(S) \oplus_{j=1}^n \langle (\phi_+ - \vec{\phi}_- U)\hat{e}_j^\top \rangle & \to & \mathscr{R}(S) \oplus_{j=1}^n \langle (\phi_+ + \vec{\phi}_- U)\hat{e}_j^\top \rangle \\ f + (\vec{\phi}_+ - \vec{\phi}_- U)\vec{k}^\top & \to & Sf + (\vec{\phi}_+ + \vec{\phi}_- U)\vec{k}^\top \ \forall g \in \mathscr{D}(S), \vec{k} \in \mathbb{C}^n \end{array} \tag{3.40}$$

*where $\vec{\phi}_\pm = \begin{pmatrix} \phi_\pm^1 & \ldots & \phi_\pm^n \end{pmatrix}$ and $\hat{e}_j^\top = (0, \ldots, 0, \overset{(j)}{1}, 0 \ldots, 0)^\top$.*

# Chapter 4

# Sobolev spaces and weak derivative

In mathematical physics, the Hamiltonians and other functions are usually defined in terms of differential operators and a suitable Hilbert space theory in this scenario is required. The Sobolev spaces accomplish this issue, with the added advantage of extending the concept of derivative beyond the usual sense, expanding to a space with functions usually not derivable everywhere.

In the chapter after this one we will apply Cayley's method for finding self-adjoint extensions to the hamiltonian and Laplacian operators. Since they are both differential operators, we will firstly further increase their domains by using derivatives not in the "normal" sense, but in the *weak sense*:

**Definition 4.1.** *Let $f$ be a function in the Lebesgue space $L^1([a,\ b])$. Then $g \in L^1([a,\ b])$ is a* weak derivative *(or* derivative in the weak sense*) of $f$ if*

$$\int_a^b g(x)h(x)dx = -\int_a^b f(x)h'(x)dx \; \forall h \in C^\infty([a,\ b]),\ h(a) = h(b) = 0. \tag{4.1}$$

*To generalise to n dimensions, let $f \in L^1_{loc}(\Omega)$, the space of locally integrable functions for an open set $\Omega \in \mathbb{R}^n$. Then $g$ is the $\alpha^{th}$ weak derivative of $f$, where $\alpha$ is a multi-index, if*

$$\int_\Omega gh = (-1)^{|\alpha|} \int_\Omega g D^\alpha h \; \forall h \in C_c^\infty(\Omega) \tag{4.2}$$

*where $C_c^\infty(\Omega)$ is the space of inginitely differentiable functions with compact support (domain without kernel) in $\Omega$, and*

$$D^\alpha h = \frac{\partial^{|\alpha|} h}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}. \tag{4.3}$$

Weak derivatives are unique up to a set of measure zero, and obviously the weak derivative of a function differentiable in the standard sense is equal to its standard derivative of the same multi-index. The space of functions with weak derivatives we will use is called the Sobolev space:

**Definition 4.2.** *. Let $k \in \mathbb{N}$. The Sobolev space $W^{k,p}(\Omega)$ is defined as the set of all functions $f$ defined on $\Omega$ such that, for every multi-index $\alpha$ with $|\alpha| \leq k$, the mixed partial derivative*

$$f^{(\alpha)} = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}} \tag{4.4}$$

*exists in the weak sense and is in $L^p(\Omega)$.*

Note that, given this definition of the Sobolov space, the derivative of index zero (that is, the function itself) must belong to $L^p(\Omega)$ too, and therefore $W^{k,p}(\Omega) \subset L^p(\Omega)$. The weak derivative of $f$ is usually written as $D^\alpha f$, but since we will use the weak sense exclusively, for the rest of this and the following sections any derivative notation, be it $f'$ or $df/dx$, will refer to the weak derivative unless stated otherwise.

Since in Quantum Physics we are interested in the integrability of $(f, f) = \int_\Omega |f|^2$, we will use the simplified notation $H^k = W^{k,2}$.

A problem presents to us: *weak funuctions*, that is, functions $f \in H^k(\Omega) \setminus C^k(\Omega)$, are defined only up to a subset of measure zero, and since $\partial\Omega$, the boundary of $\Omega$, is a subset of measure of $\Omega$, then weak functions can be redefined on the boundary without changing the function as an element in $H^k(\Omega)$, so a priori we cannot use the restriction to $\partial\Omega$ of $f$ to ascertain properties of $f$ in $\Omega$ - for instance, if $\Omega$ is the real interval $[a,\ b]$, then it seems we may not be able to use integration by parts to calculate $(f,\ g') = [fg]_a^b - (f',\ g)$. In reality, we can approximate $f$ by a sequence $(f_n)$ in $C^k(\partial\Omega)$, and define the restriction $f_{|\partial\Omega}$ as the limit of the sequence $f_{n|\partial\Omega}$. To prove that, we make use of the Trace Theorem for Sobolev Spaces:

**Theorem 4.3.** *Consider the Sobolev space $H^k(\Omega)$. Let* Tr *be the* trace operator, *defined as*

$$\begin{aligned} \mathrm{Tr} : C^k(\bar{\Omega} \cap H^k(\Omega) &\to L^2(\partial\Omega) \\ f &\to f_{|\partial\Omega} \,. \end{aligned} \tag{4.5}$$

*Then:*

1. *There exists a constant $K > 0$ such that*

$$||\,\mathrm{Tr}\, f||_{L^2(\partial\Omega)} \leq K||f||_{H^k(\Omega)}. \tag{4.6}$$

2. Tr *admitts a continuos extension* $\widetilde{\mathrm{Tr}}$,

$$\mathrm{Tr} : H^k(\Omega) \to L^2(\partial\Omega) \tag{4.7}$$

*defined everywhere on $H^k(\Omega)$.*

*Then the restriction or trace $f_{|\partial\Omega}$ of a functuion $f \in H^k\Omega$ can be defined as $\widetilde{\mathrm{Tr}} f$.*

*Proof.* Property 2 results from $C^\infty(\bar{\Omega})$ being dense in $H^k(\Omega)$ [2] and and therefore $C^\infty(\bar{\Omega})$ too, which as we showed back in chapter 2 means the operator can indeed be extended to $H^k(\Omega)$. Proving property 1 is complex and will not be done here, although a multitude of different methods for doing so can be found at [3] and [4]. The final statement can then be proved by considering a sequence of functions $(f_n)$ in $C^k(\bar{\Omega})$ that converge to $f$ in the norm of $H^k(\Omega)$. Then property 2 suffices to ensure that the sequence $f_{n|\partial\Omega}$ will converge in $L^k(\partial\Omega)$ and we can define

$$f_{|\partial\Omega} = \lim n \to \infty f_{n|\partial\Omega}. \tag{4.8}$$

□

With the trace theorem in mind, we can proceed to the practical applications of Cayley's method on the hamiltonian and the laplacian operators, with the certainty that usage of the integration in parts in $(f,\ g') = [fg]_a^b - (f',\ g)$ is valid $\forall f, g \in H^1[a,\ b]$.

# Chapter 5

# Particular examples

Remember that in this chapter any derivative notation, be it $f'$ or $df/dx$, will refer to the weak derivative, unless explicited otherwise.

## 5.1 Hamiltonian: $S = i\frac{d}{dx}$

### 5.1.1 Defining the domain - boundary conditions

First we need to define a domain where the hamiltonian operator, $S = i\frac{d}{dx}$, is symmetric, that is, where $S \subset S*$. We will consider the hermitian space $H = L^2[a,\ b]$ and, given the derivative nature of the hamiltonian operator, we will also sart with the obvious $\mathscr{D}(S) \in H^1[a,\ b]$. Then, $\forall f,\ g \in \mathscr{D}(S)$,

$$(Sf,\ g) = \int_a^b if'(x)\overline{g(x)}dx = i(f(b)\overline{g(b)} - f(a)\overline{g(a)}) - i\int_a^b f(x)\overline{g'(x)}dx =$$

$$= i(f(b)g(b) - f(a)g(a)) + \int_a^b f(x)\overline{ig'(x)}dx = i(f(b)\overline{g(b)} - f(a)\overline{g(a)}) + (f,\ Sg). \quad (5.1)$$

Here we clearly see that the condition for symmetry is $(f(b)\overline{g(b)} - f(a)\overline{g(a)}) = 0$. The boundary condition that gives this result is $\exists\omega \in [0,\ 2\pi)\ f(a) = e^{i\omega}f(b)\ \forall f \in \mathscr{D}(S)$, but we will add another condition: Since we want the adjoint $S^*$ to behave the same as $S$ albeit in all of $\mathscr{D}(S^*)$ (else we both hamper our chances of finding self-adjoint extensions and produce results not relevant to Quantum Physics), we will also require that $S^*g = ig'$ not only $\forall g \in \mathscr{D}(S)$, but also $\forall g \in H$. This will require that, $\forall f \in \mathscr{D}(S)$ and $\forall g \in H$,

$$(Sf,\ g) = i(f(b)\overline{g(b)} - f(a)\overline{g(a)}) + (f,\ S^*g) \quad (5.2)$$

and since we have to achieve it only by limiting $\mathscr{D}(S)$ and not $\mathscr{D}(S^*) = H = H^1[a,\ b]$, the boundary condition becomes $f(a) = f(b) = 0\ \forall f \in \mathscr{D}(S)$.

Note that if, instead of $H^2[a,\ b]$, we set $H = H^1[a,\ \infty)$, then $\mathscr{D}(S)$ is only limited by the condition $f(a) = 0$, since $\lim_{b\to\infty} fb = 0$ by the fact that $H^1[a,\ \infty) \subset L^2[a,\ \infty)$, and the same if $H = H^1(-\infty,\ b]$. If $H = H^1(\mathbb{R})$ then $\mathscr{D}(S) = \mathscr{D}(S^*) = H$, which alongside the operator's symmetry means that $S$ is already self-adjoint.

There are, then, two different cases to study - $H = H^1[0,\ 1]$ (since the particular finite values of $a$ and $b$ are irrelevant to the study) and $H = H^1[0,\ \infty)$.

### 5.1.2 Case $H = H^1[0,\ 1]$

As we've proven before, here $S$ and $S^*$ are both defined as $i\frac{d}{dx}$ in their respective domains, which are

$$\begin{aligned} \mathscr{D}(S) &= \{f \in H^1[0,\ 1] \mid f(0) = f(1) = 0\} \\ \mathscr{D}(S^*) &= H^1[0,\ 1]. \end{aligned} \tag{5.3}$$

Now we start Cayley's method by finding the deficiency subspaces of $S$:

$$\begin{aligned} D_\pm = \mathrm{Ker}(S^* \mp i) &= \mathrm{Ker}(i\frac{d}{dx} \mp i) \\ f_\pm \in D_\pm \iff f'_\pm \mp f_\pm = 0 &\iff f_\pm(x) = ke^{\pm x},\ k \in \mathbb{C}. \end{aligned} \tag{5.4}$$

It is clear from this last equation that $d_+ = d_- = 1$, and so $S$ *does* have self-adjoint extensions. Now, following (3.30), these can be labeled by $\theta \in [0,\ 2\pi)$ and will be

$$A_\theta(f + k(e^x - e^{i\theta - x})) = if' + ik(e^x + e^{i\theta - x})\ \forall f \in \mathscr{D}(S),\ k \in \mathbb{C}. \tag{5.5}$$

In fact, since $A_\theta(k(e^x - e^{i\theta-x})) = ik(e^x + e^{i\theta-x}) = i\frac{d}{dx}(k(e^x - e^{i\theta-x}))$, we can simplify it to

$$\begin{aligned} A_\theta :\ \mathscr{D}(S) \oplus \langle e^x - e^{i\theta - x}\rangle &\to \mathscr{R}(S) \oplus \langle e^x + e^{i\theta - x}\rangle \\ g &\to ig'. \end{aligned} \tag{5.6}$$

In particular, note how $\mathscr{D}(A_0) \setminus \mathscr{D}(S) = \langle \sinh \rangle$ and $\mathscr{R}(A_0) \setminus \mathscr{R}(S) = \langle \cosh \rangle$, and the same for $A_\pi$ except for exchanging sinh and cosh.

### 5.1.3 Case $H = H^1[0,\ \infty)$

As always, $S$ and $S^*$ are both defined as defined as $i\frac{d}{dx}$ in their respective domains, this time

$$\begin{aligned} \mathscr{D}(S) &= \{f \in H^1[0,\ \infty) \mid f(0) = 0\} \\ \mathscr{D}(S^*) &= H^2[0,\ \infty). \end{aligned} \tag{5.7}$$

Howver, we find ourselves with a new problem when calculating the deficiency subspaces:

$$\begin{aligned} D_\pm = \mathrm{Ker}(S^* \mp i) = \mathrm{Ker}(i\frac{d}{dx} \mp i) & \\ f_\pm \in D_\pm \iff f'_\pm \mp f_\pm = 0 \iff f_-(x) &= ke^{-x},\ k \in \mathbb{C} \\ f_+(x) &= 0. \end{aligned} \tag{5.8}$$

The result $D_+ = \{0\}$ is a consequence of the functions $ke^x \notin L^2[0,\infty)$ except for $k = 0$, and since $L^2[0,\infty) \ni H^2[0,\ \infty$, then $ke^x \notin L^1[0,\ \infty) \implies ke^x \notin H^2[0,\ \infty)$.

So in this case, $d_+ = 0$ and $d_- = 1$. Since $d_+ \neq d_-$, by Theorem 3.6, the hamiltonian defined in this domain has no self-adjoint extensions. It's the same when $H = H^1(-\infty,\ 0]$, except that $D_- = \{0\}$ and $D_+ = \{f(x) = ke^x \mid k \in \mathbb{C}\}$.

## 5.2 Laplacian: $S = -\frac{d^2}{dx^2}$

### 5.2.1 Domain definitions

Just like with the hamiltonian, we start on the same space $H = L^2[a,\ b]$, and we first need to see which boundary conditions, this time in $\mathscr{D}(S) \in H^2[a,\ b]$, make the Laplacian a symmetric operator:

$$\begin{aligned}(Sf,\ g) &= -\int_a^b f''(x)\overline{g(x)}dx = -f'(b)\overline{g(b)} + f'(a)\overline{g(a)} + \int_a^b f'(x)\overline{g'(x)}dx = \\ &= -f'(b)\overline{g(b)} + f'(a)\overline{g(a)} - f(b)\overline{g'(b)} + f(a)\overline{g'(a)} - \int_a^b f(x)\overline{g''(x)}dx = \\ &= -f'(b)\overline{g(b)} + f'(a)\overline{g(a)} - f(b)\overline{g'(b)} + f(a)\overline{g'(a)} + (f,\ Sg). \end{aligned} \tag{5.9}$$

The requirement $[f'(x)\overline{g(x)} + f(x)\overline{g'(x)}]_a^b = 0$, then, is achieved by any of the following boundary conditions $\forall f \in \mathscr{D}(S)$:

1. $f(a) = f(b) = 0$, the Dirichlet condition.
2. $f'(a) = f'(b) = 0$, the Neuman condition.
3. $f(0) = f(1)$ and $f'(a) = f'(b)$, the periodic condition.
4. $cf(a) - df'(a) = cf(b) + df'(b) = 0,\ a, b \in \mathbb{R} \setminus \{0\}$, the Robin condition.
5. $f(a) - e^{i\theta} f(b) = f'(a) - e^{i\theta} f'(b) = 0,\ \theta \in [0,\ 2\pi)$, the Born-von Karman condition.

For it to be relevant to Quantum Physics, we will also impose, like before, that the adjoint of $S$ behave in $\mathscr{D}(S^*) = H^2[a,\ b]$ as it does in $\mathscr{D}(S)$, that is, $S^*g = -g''\ \forall g \in H^2[a,\ b]$. This further restricts the boundary conditions, as $[f'(x)\overline{g(x)} + f(x)\overline{g'(x)}]_a^b = 0$ must hold $\forall f \in \mathscr{D}(S)$ and $\forall g \in H^2[a,\ b]$. The only way to achieve this is by combining Dirichlet and Neuman's conditions:

$$\mathscr{D}(S) = \{f \in H^2[a,\ b] \mid f(a) = f(b) = f'(a) = f'(b) = 0\}. \tag{5.10}$$

Since $f \in H^2 \implies f,\ f' \in L^2$, here too replacing one of the extremes of $[a,\ b]$ to minus or plus infinity gets rid of the condition that $f$ and $f'$ be zero in that limit, since that's a property inherent to $L^2$. And setting the hermitan space to $H = H^2[\mathbb{R}]$ renders all boundary conditions unnecessary and results in $\mathscr{D}(S) = H^2[a,\ b]$, so that $S$ is already self-adjoint.

### 5.2.2 Case $H = H^2[0,\ 1]$

$S$ and $S^*$ are both defined as $-\frac{d^2}{dx^2}$ in ther respective domains, which are

$$\begin{aligned}\mathscr{D}(S) &= \{f \in H^2[0,\ 1] \mid f(0) = f(1) = f'(0) = f'(1) = 0\} \\ \mathscr{D}(S^*) &= H^2[0,\ 1]. \end{aligned} \tag{5.11}$$

We then find the deficiency subspaces:

$$\begin{aligned} D_\pm &= \operatorname{Ker}(S^* \mp i) = \operatorname{Ker}(-\frac{d}{dx} \mp i) \\ f_\pm &\in D_\pm \iff f''_\pm \pm i f_\pm = 0 \iff f_\pm(x) = a e^{(i\mp 1)x} + b e^{-(i\mp 1)x},\ a, b \in \mathbb{C} \end{aligned} \tag{5.12}$$

Since $f_+$ and $f_-$ both vary depending on two complex constants each, we have $d_+ = d_- = 2$. We now choose the bases $\{e_1^+ = e^{(i-1)x},\ e_2^+ = e^{-(i-1)x}\}$ for $D_+$ and $e_1^- = \{e^{(i+1)x},\ e_2^- = e^{-(i+1)x}\}$ for $D_-$, and then for any unitary $2 \times 2$ matrix $U$, as defined in (3.33), we can define the isometry

$$\begin{aligned} V_U :\ D_+ &\to D_- \\ a e_1^+ + b e_2^+ &\to \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U \begin{pmatrix} a \\ b \end{pmatrix} \end{aligned} \tag{5.13}$$

and using this isometry to extend the Cayley transform, the self-adjoint extension will be defined, as shown in (3.35), in

$$\begin{aligned} \mathscr{D}(A_U) &= \mathscr{D}(S) \oplus \langle e_1^+ - \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ e_2^+ - \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rangle \\ \mathscr{R}(A_U) &= \mathscr{R}(S) \oplus \langle e_1^+ + \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ e_2^+ + \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rangle \end{aligned} \tag{5.14}$$

and, since $-\frac{d^2}{dx^2} e_j^+ = i e_j^+$, $j \in \{1,\ 2\}$ and $-\frac{d^2}{dx^2} \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U = -i \begin{pmatrix} e_1^- & e_2^- \end{pmatrix} U$, we can write $A_U$ simply as

$$\begin{aligned} A_U : \mathscr{D}(A_U) &\to \mathscr{R}(A_U) \\ f &\to -f''. \end{aligned} \tag{5.15}$$

### 5.2.3 Case $H = H^2[0,\ \infty)$

We start like above, and find the deficiency subspaces:

$$\begin{aligned} D_\pm &= \operatorname{Ker}(S^* \mp i) = \operatorname{Ker}(-\frac{d}{dx} \mp i) \\ f_\pm &\in D_\pm \iff f''_\pm \pm i f_\pm = 0 \iff f_\pm(x) = k e^{-(1\mp i)x}\ k \in \mathbb{C}. \end{aligned} \tag{5.16}$$

Since the only exponentials in $H = H^2[0,\ \infty)$ are those with a negative real part on their exponential coefficient, this time we have $d_+ = d_- = 1$, so unlike the Hamiltonian, the Laplacian *does* have self-adjoint extensions from this domain. We choose the bases $\{e^{-(1-i)x}\}$ and $\{e^{-(1+i)x}\}$ for $D_+$ and $D_-$, respectively, and define an isometry between them depending on $\theta \in [0,\ 2\pi)$:

$$\begin{aligned} V_\theta :\ D_+ &\to D_- \\ k e^{-(1-i)x} &\to k e^{i\theta - (1+i)x}. \end{aligned} \tag{5.17}$$

And, as always, use it to extend the Cayley transform and recover the self-adjoint extension

$$\begin{aligned} A_\theta :\ \mathscr{D}(S) \oplus \langle e{-}(1 - i^x - e^{-i\theta-(1+i)x}\rangle &\to \mathscr{R}(S) \oplus \langle e^{-(1-i)x} + e^{i\theta-(1+i)x}\rangle \\ f &\to -f''. \end{aligned} \tag{5.18}$$

The case $H = H^2(-\infty,\ 0]$ is the same, except with $\{e^{(1-i)x}\}$ and $\{e^{(1+i)x}\}$ as the bases of $D_+$ and $D_-$ instead.

# Chapter 6

# Conclusions

It is worth repeating that even though we have Cayley's is only one of multiple methods of finding self-adjoint extensions, Theorem 3.7 clearly states that, since there is a bijection between such extensions and the isometries with which to extend the Cayley transform, then through Cayley's method we can find *all* the self-adjoint extensions of a given operator, as long as we can find all the equivalent isometries.

It might have stood out during chapter 5 that we never formulated explicitedly the action of the Cayley transform of the unextended hamiltonian and laplacian, instead only doing so for the isometry between $D_+$ and $D_-$ that is part of the unitary extension of the transform. That is instentional, as the Cayley transform, which we remind is defined as $V = (S - iI)(S + iI)^{-1}$, can sometimes be far from simple when working with unbounded operators due to its inverse component, and as we showed, it is not necessary at all in order to find the extensions. In this sense, the unextended Cayley transform is more of a support than it is a tool; its usage in the method is only tangential.

Lastly, through chapter 5 we choose boundary conditions more limiting than those strictly necessary to make the hamiltonian and laplacian symmetric operators, alluring briefly to the fact that it was in the interest of the results being relevant to Quantum Physics. This is mostly true - much like in simpler mechanics, "non-physical" solutions to differential equations are usually tossed aside, in Quantum Physics defining operators piecewise is not a good practice unless we are treating the domain like a spectrum. After all, defining the hamiltonian as something *not* $i\frac{d}{dx}$ would make it *not* the hamilatonian in that domain. For that purpose we specified that both $S^*$ be the same differential operator in all of its domain, and that said domain $\mathscr{D}(S^*)$ be the upper limit for extensions of $S$ that still behaved as the same differnecial operator, as doing so guarantees that any self-adjoint extension $A$, by virtue of $A = A^* \in S^*$, would also be defined as the same differential operator in all $\mathscr{D}(A)$, and in particular, in $\mathscr{D}(A) \setminus \mathscr{D}(S)$. Aditionally, choosing too generic a boundary condition for $\mathscr{D}(S)$ would have resulted, in some cases, in $S$ being already self-adjoint, and thus of no interest to work in.

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