Bachelor's Thesis

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On Self-adjointness in Quantum Theory

Faculty of Mathematics, Informatics and Statistics
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Über Selbstadjungiertheit in der Quantenmechanik

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Contents

1 Introduction

Quantum mechanics is a fundamental theory in physics which describes the behavior of nature at and below the scale of atoms. In nonrelativistic quantum mechanics, a particle has wave-like properties and can be described by a wave function ψ. The central object of quantum mechanics, independent of its interpretation, is the so-called Schrödinger equation. It governs how the wave function evolves in space and time. This differential equation is not only the main ingredient of the theory but turns out to give rise to interesting mathematical structure.
A solution of the differential equation with a given initial state of the system $\psi(x)$ at a starting point in time can be written as $\psi(x,t) = U(t)\psi(x)$. From a physical standpoint, by demanding different properties to this solution, we shall obtain a strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$ which is called the time evolution group. We shall see that every such group can be uniquely characterised by a generator. Both of these objects are potentially difficult to handle due to their mathematical properties. In order to give mathematical meaning to them we will use tools from functional analysis.
The outline of this thesis is as follows. In Section 2 we shall state the Schrödinger equation and formulate mathematical requirements on a solution based on a physical motivation. These provide the formal characterisation of a time evolution group which will lead to its generator. Defining properties of this generator will be given in Theorem (2.8). Section 3 covers the operator theory needed to study the found properties in a more explicit setting. Criteria for the so-called self-adjointness of an operator are captured in Theorem (3.8) and (3.10), which can be used to mathematically characterise the generator.
Conversely, for a given Hamilton operator H of a system, we want to obtain existence and uniqueness of solutions for the Schrödinger equation and find the corresponding time evolution group $(U(t))_{t\in\mathbb{R}}$ with generator H. This will be done in Chapter 4 with the Hille-Yosida Theorem (4.1). In Section 5, we consider a special case of the preceding work to study the Schrödinger equation from yet another angle. The main result of this chapter will be the Stone's Theorem (5.9). Lastly, we apply these results in Section 6 when we discuss a number of physically relevant examples while developing an important tool to study the self-adjointness of sums of operators, the Kato-Rellich Theorem (6.4).
To conclude the discussion of the time evolution and self-adjointness in quantum mechanics, we will give an outlook on possible extensions of this theory and the current research topics.

2 The Schrödinger equation

2.1 The Schrödinger equation

In order to understand the mathematical structure of quantum mechanics, we state the two main ingredients. The fundamental object is the time-dependent Schrödinger equation which determines how the wave function ψ of a nonrelativistic quantum particle behaves:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = H\psi(x,t) \tag{2.1}$$

where H is the so-called Hamilton operator, or short, Hamiltonian. A discussion about the domain of this operator will follow.
A physically common example of a Hamiltonian is given by $H = -\Delta + V(x)$ where $\Delta\psi = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}\psi$ denotes the Laplace-operator with respect to the spatial variables and $V(x)$ is a potential which is constant in time. Physically, it coincides with the total energy of a particle in a potential. From now on we will use the unit $\hbar = 1$.
Secondly, by Born's interpretation of the wave function ψ, the squared norm $|\psi(x,t)|^2\, d^3x$ gives the probability of finding the particle at position x at time t.
In conclusion, for a specific initial state $\psi_0(x) \in \mathcal{H}$ of a particle, more accurately, a probability distribution at a starting time $t = 0$, the time evolution of the wave function is characterised by

$$\begin{cases} i\dfrac{\partial\psi(x,t)}{\partial t} = H\psi(x,t) \\ \psi(x,0) = \psi_0(x). \end{cases} \tag{2.2}$$

To make sense of this, let us translate the problem into a mathematical framework.

2.2 Initial value problem

By Born's rule, $|\psi(x,t)|^2$ is desired to be a probability measure on $\mathbb{R}^n$ for each $t \in \mathbb{R}$, so we choose $L^2(\mathbb{R}^n, \mathbb{C})$ as our candidate space for $\psi(x,t)$ as a function of x for fixed t. The function space $\mathcal{H} := L^2(\mathbb{R}^n, \mathbb{C})$ is a Hilbert space when equipped with the inner product

$$\langle f, g\rangle := \int_{\mathbb{R}^n} \overline{f(x)} g(x)\, dx. \tag{2.3}$$

The inner product induces a norm $\|\cdot\| := \sqrt{\langle\cdot,\cdot\rangle}$ on $\mathcal{H}$ with respect to which the space is complete, see [1, Sec. 5.1].
In general, an initial value problem (IVP) on an arbitrary Hilbert space $\mathcal{H}$ consists of a differential equation and a domain of initial values $\mathrm{dom}(\mathrm{IVP}) \subseteq \mathcal{H}$. Since the Schrödinger equation is a differential equation of first order, we will only cover this case here.
For a given mapping $F : \mathrm{dom}(F) \to \mathcal{H}$ on $\mathrm{dom}(F) \subseteq \mathcal{H} \times \mathbb{R}$ and $\psi_0 \in \mathrm{dom}(\mathrm{IVP})$ the IVP reads

$$\begin{cases} \dfrac{d\psi(t)}{dt} = F(\psi, t) \\ \psi(0) = \psi_0(x) \end{cases} \tag{IVP}$$

where $\psi : \mathbb{R} \to \mathcal{H}$. The initial value problem is considered well-defined if for any initial condition $\psi_0 \in \mathrm{dom}(\mathrm{IVP})$, there is a unique solution $\psi(t)$ with $\psi(t) \in \mathrm{dom}(\mathrm{IVP})$ at all times $t \in \mathbb{R}$.
The Schrödinger equation (2.4) is an initial value problem where $F(\psi, t) := -iH\psi(t)$ for a possibly unbounded operator $H : \mathrm{dom}(H) \to \mathcal{H}$ on $\mathrm{dom}(H) \subseteq \mathcal{H}$.
For a solution $\psi : \mathbb{R} \to \mathcal{H}$ of (2.4) with the initial state $\psi_0 \in \mathcal{H}$, we want to write $\psi(t) = U(t)\psi_0$. For each time $t \in \mathbb{R}$, we may view $U(t)$ as a map from $\mathcal{H}$ onto $\mathcal{H}$. When we think of $\psi(x, \cdot)$ as a vector-valued function $\psi : \mathbb{R} \to \mathcal{H}, t \mapsto \psi(t)$, we can understand (2.2) as an ordinary linear differential equation

$$i\frac{d\psi(t)}{dt} = H\psi(t) \text{ with the initial condition } \psi(0) = \psi_0. \tag{2.4}$$

A solution of this equation is a differentiable function $\psi : I \to \mathcal{H}$ on a nontrivial open interval $I \in \mathbb{R}$ with $0 \in I$ that satisfies

(1) $\forall t \in I : \psi(t) \in \mathrm{dom}(H)$,

(2) $\forall t \in I : i\dfrac{d}{dt}\psi(t) := \lim\limits_{h\to 0} i\dfrac{\psi(t+h)-\psi(t)}{h} = H\psi(t)$,

(3) $\lim_{t\to 0}\psi(t) = \psi_0$.

Here, we are interested in global solutions where $I = \mathbb{R}$. Heuristically, this motivates a "solution" of the form $\psi(t) = e^{-iHt}\psi_0$ and $U(t) = e^{-iHt}$. However, to define and deal with such an object mathematically in strict generality will turn out to require great care.
The well-definedness of the exponential of a finite-dimensional matrix already requires various preconditions. Here, the operator H might even be unbounded. A key part of this thesis will be to find ways to make sense of a similar expression for certain operators H.
We convert the physical motivation from Section 2.1 into mathematical expressions: By nature of equation (2.2), we imply that the time evolution should not only be unique but also linear, that is $U(t+s)\psi = U(t)U(s)\psi$ for all $t, s \in \mathbb{R}$ and $U(0) = I$, where I is the identity operator on $\mathcal{H}$. It should not make a difference to consider a passed time $t+s$ at once or split up into sections. We refer to this as group property (P1).
Furthermore, Born's interpretation demands $|\psi(x,t)|^2$ to represent a probability distribution in space at all times $t \in \mathbb{R}$. Hence, we want the norm $\|\psi(t)\|$ to be constant in $t \in \mathbb{R}$: $\|U(t)\psi_0\| = \|\psi(t)\| = \|\psi(0)\| = \|\psi_0\|$. This will be called group property (P2).
Since we want to take some kind of derivative with respect to the time variable t of the solution, it seems reasonable to require at least continuity which will be point (P3). Later we will have to talk about further regularity to also be able to treat derivatives. This discussion motivates the following definition of a so-called strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$.

2.3 Strongly continuous unitary groups

Although, we will have in mind $\mathcal{H} = L^2$, in this section we may also take $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ to be a general Hilbert space with the norm $\|\cdot\| = \sqrt{\langle\cdot,\cdot\rangle}$.

Definition 2.1. A bounded operator $U : \mathcal{H} \to \mathcal{H}$ which is onto is called unitary if and it is isometric, i.e. if for all $\psi \in \mathcal{H} : \|U\psi\| = \|\psi\|$, and onto.

With the polarization identity, [2, Thm 0.32], i.e.,

$$\langle\varphi,\psi\rangle = \frac{1}{4}\Big[\|\varphi+\psi\|^2 - \|\varphi-\psi\|^2 - i\big(\|\varphi+i\psi\|^2 - \|\varphi-i\psi\|^2\big)\Big] \tag{2.5}$$

we see that any unitary operator U satisfies $\langle U\varphi, U\psi\rangle = \langle\varphi,\psi\rangle$ for all $\varphi, \psi \in \mathcal{H}$.
The above discussion motivates the following definition.

Definition 2.2. A strongly continuous unitary one-parameter group $(U(t))_{t\in\mathbb{R}}$ is a family of linear operators $U(t) : \mathcal{H} \to \mathcal{H}$ on $\mathcal{H}$ for each $t \in \mathbb{R}$ such that the following conditions are satisfied:

(1) $U(t+s) = U(t)U(s)$ for all $s, t \in \mathbb{R}$ and $U(0) = I$

(2) $\|U(t)\psi\| = \|\psi\|$ for all $t \in \mathbb{R}, \psi \in \mathcal{H}$

(3) $t \mapsto U(t)\psi$ is continuous for each $\psi \in \mathcal{H}$

Note that this object $(U(t))_{t\in\mathbb{R}}$ satisfies the basic requirements (P1), (P2) and (P3) mentioned in Section 2.2.
From (1) we deduce that each $U(t)$ is invertible on $\mathcal{H}$ with the inverse $U(-t)$ since $U(t)U(-t) = U(-t)U(t) = U(0) = I$. For further discussions about unitary groups we always consider strongly continuous unitary one-parameter groups, even when some of these properties are not explicitly mentioned.

Lemma 2.1. For each $t \in \mathbb{R}$ the operator $U(t)$ in Definition (2.2) is indeed a unitary operator according to Definition (2.1).

Proof. Let $t \in \mathbb{R}$. For all $\varphi \in \mathcal{H}$ take $\psi = U(-t)\varphi$, then $U(t)\psi = \varphi$. Therefore, U is onto. By (2) in Definition (2.2) U is isometric. Hence, it is unitary. □

Now we want to connect the unitary group from Definition (2.2) with the Schrödinger equation.

2.4 Generator of a unitary group

If $(U(t))_{t\in\mathbb{R}}$ is a strongly continuous unitary group, the function $U(t)\psi$ fulfills the desired properties (P1), (P2) and (P3) for a solution. The only missing requirement is the connection to the Schrödinger equation, namely

$$i\frac{d}{dt}\big(U(t)\psi\big) = HU(t)\psi \quad \text{for all } \psi \in \mathcal{H} \tag{2.6}$$

with the Hamiltonian $H : \mathrm{dom}(H) \to \mathcal{H}$ on its domain $\mathrm{dom}(\mathcal{H})$. Remember that this operator is possibly, and in many relevant physical settings in fact, unbounded. The crucial point is technical, however important: The domain $\mathrm{dom}(H)$ may not be the whole Hilbert space. The initial value problem is considered well-defined if for any initial condition $\psi \in \mathrm{dom}(H)$, there is a unique solution $\psi(t)$ with $\psi(t) \in \mathrm{dom}(H)$ at all times $t \in \mathbb{R}$. This means that $\mathrm{dom}(H)$ must be invariant under every time evolution operator $U(t)$, i.e.

$$U(t)\,\mathrm{dom}(H) = \mathrm{dom}(H) \quad \text{for all } t \in \mathbb{R}. \tag{2.7}$$

However, (P3) is not enough to provide this differentiability property. Rather, the requirement leads to the definition of a new object, the so-called generator of a unitary group. Its domain is chosen to make sense of the initial value problem as we will see later on.

Definition 2.3. A densely defined operator $A : \mathrm{dom}(A) \to \mathcal{H}$, that means $\mathrm{dom}(A) \subseteq \mathcal{H}$ is dense, is called generator of a unitary group $(U(t))_{t\in\mathbb{R}}$ if the following holds:

(1) $\mathrm{dom}(A) = \left\{\psi \in \mathcal{H} \mid \lim\limits_{h\to 0} \dfrac{U(t+h)\psi - U(t)\psi}{h} \text{ exists for all } t \in \mathbb{R}\right\}$

(2) $i\dfrac{d}{dt}U(t)\psi := i\lim\limits_{h\to 0}\dfrac{U(t+h)\psi - U(t)\psi}{h} = AU(t)\psi$ for all $t \in \mathbb{R}, \psi \in \mathrm{dom}(A)$

where the limit is always with respect to the norm on $\mathcal{H}$.

We will successively work out what this generator has to offer. To make these identifications, we assume for now that the IVP (2.4) is well-defined, i.e., that there is a unique solution for all allowed initial states in some set we want to identify. This provides a strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$.
The question arises whether every unitary group has a generator and if so, whether there are multiple ones. We follow a similar approach as the one in [3, Sec. 7.4] but instead of contracting semi-groups, here we are discussing unitary groups. Let $(U(t))_{t\in\mathbb{R}}$ be a strongly continuous unitary group defined as in Definition (2.2), then there is an obvious candidate, defined by $H : \mathrm{dom}(H) \to \mathcal{H}$,

$$\begin{cases} \mathrm{dom}(H) := \left\{\psi \in \mathcal{H} \mid \lim_{t\to 0} \dfrac{U(t)\psi - \psi}{t} \text{ exists}\right\} \\ H\psi := i \lim_{t\to 0} \dfrac{U(t)\psi - \psi}{t}. \end{cases} \tag{2.8}$$

This is the so-called infinitesimal generator. Note that we are demanding the differentiability property as seen in the definition of a generator just for $t = 0$. We will prove that this is enough for H to satisfy the requirements in Definition (2.3).
Since the limit of equation (2.8) exists for $\psi \in \mathrm{dom}(H)$ and $U(t)$ is linear, H is a linear operator. We see that the domain of a possible generator, given in Definition (2.3) (1), is contained in $\mathrm{dom}(H)$ since the condition is fulfilled in particular for $t = 0$. In the following, we check that the inverse inclusion and the equality in (2) holds for all $t \in \mathbb{R}$ by using the group properties of $U(t)$. Then, if the domain is dense in $\mathcal{H}$, H is a generator of $(U(t))_{t\in\mathbb{R}}$.

Theorem 2.2 (Differential properties of unitary groups)**.** Let H be defined as in (2.8), $t \in \mathbb{R}$ and $\psi \in \mathrm{dom}(H)$, then

(1) $U(t)\psi \in \mathrm{dom}(H)$,

(2) $U(t)H\psi = HU(t)\psi$,

(3) the mapping $t \mapsto U(t)\psi$ is differentiable in $\mathbb{R}$,

(4) $i\dfrac{d}{dt}U(t)\psi := i \lim_{h\to 0} \dfrac{U(t+h)\psi - U(t)\psi}{h} = HU(t)\psi$

Proof. Let $t \in \mathbb{R}$ and $\psi \in \mathrm{dom}(H)$.

(1) If $t = 0$, $U(0)\psi = \psi \in \mathrm{dom}(H)$. Otherwise, by the group property (1) in Definition (2.2)

$$\lim_{s\to 0} \frac{U(s)U(t)\psi - U(t)\psi}{t} = \lim_{s\to 0} \frac{U(t)U(s)\psi - U(t)\psi}{t} = U(t) \lim_{s\to 0} \frac{U(s)\psi - \psi}{t} = U(t)H\psi,$$

where we used the continuity of $U(t)$ to interchange the operator with the limit. Therefore, the limit exists and $U(t)\psi \in \mathrm{dom}(H)$. This implies that $\mathrm{dom}(H)$ is a subset of the domain of a generator.

(2) We compute

$$U(t)H\psi = U(t)i\frac{d}{ds}U(s)\psi|_{s=0} = i\frac{d}{ds}U(s)U(t)\psi|_{s=0} = HU(t)\psi.$$

This implies $\|HU(t)\psi\| = \|U(t)H\psi\| = \|H\psi\|$ for all $t \in \mathbb{R}$.

(3) Let $h \neq 0$, then with (1)

$$\lim_{h\to 0}\Big(\frac{U(t+h)\psi - U(t)\psi}{h} - U(t)H\psi\Big) = \lim_{h\to 0} U(t)\Big(\frac{U(h)\psi - \psi}{h} - H\psi\Big) = 0$$

where we used again the continuity of $U(t)$. Therefore, $t \mapsto U(t)\psi$ is differentiable in all $t \in \mathbb{R}$.

(4) Combining (3) and (2), we find

$$\lim_{h\to 0} \frac{U(t+h)\psi - U(t)\psi}{h} = U(t) \lim_{h\to 0} \frac{U(h)\psi - \psi}{h} = U(t)H\psi.$$

Thus, $i\dfrac{d}{dt}U(t) = U(t)H\psi = HU(t)\psi$ exists for all $t \in \mathbb{R}$. □

Hence, if H is densely defined, then it is a generator of the unitary group $(U(t))_{t\in\mathbb{R}}$.

2.5 Properties of generators

Since H is possibly unbounded and the already mentioned heuristic idea for a unitary group $U(t) = e^{-iHt}$ is fairly complicated in a formal mathematical setting, we first need to develop some tools to efficiently study these objects.

Definition 2.4. The graph of an operator $A : \mathcal{H} \supseteq \mathrm{dom}(A) \to \mathcal{H}$ is the linear subspace

$$\Gamma(A) = \big\{(\psi, A\psi) \,|\, \psi \in \mathrm{dom}(A)\big\} \subseteq \mathcal{H} \times \mathcal{H}.$$

A linear operator A is called closed if $\Gamma(A)$ is a closed subset of $\mathcal{H}\times\mathcal{H}$ with respect to the graph norm $\|\psi\|_A := \|\psi\| + \|A\psi\|$.

The closedness in the graph norm is equivalent to the following statement: For all sequences $(\psi_n)_{n\in\mathbb{N}}$ in $\mathrm{dom}(A)$, if $\|\psi_n - \psi\| \to 0$ and $\|A\psi_n - \varphi\| \to 0$ as $n \to \infty$ for some $\psi, \varphi \in \mathcal{H}$, we have $\psi \in \mathrm{dom}(A)$ and $\varphi = A\psi$.

Theorem 2.3 (Closed graph theorem)**.** Let X, Y be Banach spaces and $A : X \to Y$ a linear operator. Then A is bounded if and only if A is closed.

Proof. See [4, Theorem III.12]. □

Therefore, every bounded linear operator that maps the whole Hilbert space $\mathcal{H}$ into itself is closed. In particular, this applies to unitary operators.
In the following section, we want to interchange a closed operator with an $\mathcal{H}$-valued integral, that is the integral of a vector- and parameter-valued function $f(x,t) = f_t(x) \in \mathcal{H}$ for each $t \in \mathbb{R}$ integrated with respect to the parameter on a compact interval. Remember that $\mathcal{H} = L^2(\mathbb{R}^n)$.

Lemma 2.4. Let $A : \mathrm{dom}(A) \to \mathcal{H}$ be a densely defined, closed linear operator with $Af(x,t)$ continuous in $t \in [a,b]$ for all such continuous $f(x,\cdot) \in \mathrm{dom}(A) \subseteq \mathcal{H}$. Then, we have

$$A\Big(\int_a^b f(x,t)\,dt\Big) = \int_a^b Af(x,t)\,dt \tag{2.9}$$

The integral is a so-called Bochner integral. We evaluate the integral over t pointwise for each $x \in \mathbb{R}^n$ and, as a result, obtain a well-defined L^2-equivalence class. We give a short sketch of the proof, however this will not be discussed further. For more details, see [5, Thm 1.2.4].

Sketch of proof. Let $f(x,\cdot) \in \mathrm{dom}(A)$ be continuous and therefore integrable for fixed $x \in \mathbb{R}^n$. Similar to Riemann integrals we can define the integral as a the limit over partitions $P = (a = t_0, t_1, \ldots, t_m = b)$ of $[a,b]$:

$$\int_a^b f(x,t)\,dt = \lim_{m\to\infty} \sum_{i=1}^m f(x,t_i^*)\Delta t_i$$

where $t_i^* \in [t_{i-1}, t_i]$ and $\Delta t_i = t_{i-1} - t_i$. The limit $m \to \infty$ is to be understood as taking the limit of the width $\Delta t_i \to 0$. Its well-definedness can be shown analogously to real Riemann integrals using the continuity of f. Since A is linear, we can pull it into a finite sum:

$$A\sum_{i=1}^m f(x,t_i^*)\Delta t_i = \sum_{i=1}^m Af(x,t_i^*)\Delta t_i$$

Interchanging A with a limit is however not trivial since it is only closed but not necessarily continuous. For this, one has to define the function $g : [a,b] \to \mathcal{H} \times \mathcal{H}, g(t) := (f(\cdot,t), Af(\cdot,t))$ and use the closedness of the operator A. We omit further details here. Taking the limit $m \to \infty$ on both sides, we obtain (2.9). $\square$

All the following integrals are in the setting such that this lemma can be applied to the closed operators $U(t)$ and, as we will see later, H. Furthermore, the fundamental theorem of calculus can be applied to these integrals in the same way as in the Riemann theory.

Theorem 2.5. Let H be defined as in Definition (2.8).

(1) The domain $\mathrm{dom}(H)$ is dense in $\mathcal{H}$.

(2) H is a closed operator.

Proof. For any $\psi \in \mathcal{H}$ define $\psi^t := \int_0^t U(s)\psi\,ds$ for $t > 0$. By property (1) in Definition (2.2) $s \mapsto U(s)\psi$ is continuous on $\mathbb{R}$, so we can differentiate the integral with respect to t. Hence

$$\begin{aligned}\lim_{t\to 0}\frac{\psi^t}{t} &= \lim_{t\to 0}\frac{1}{t}\int_0^t U(s)\psi\,ds = \lim_{t\to 0}\frac{1}{t}\Big(\int_0^{\tilde{t}} U(s)\psi\,ds|_{\tilde{t}=t} - \int_0^{\tilde{t}} U(s)\psi\,ds|_{\tilde{t}=0}\Big)\\ &= \frac{d}{dt}\Big(\int_0^t U(s)\psi\,ds\Big)|_{t=0} = U(0)\psi = \psi \quad \text{in } \mathcal{H}.\end{aligned}$$

We claim $\psi^t \in \mathrm{dom}(H)$, then we have $\dfrac{\psi^t}{t} \in \mathrm{dom}(H)$, since $\mathrm{dom}(H)$ is a linear subspace. Let $h \neq 0$, by the group property we have

$$\begin{aligned}\frac{U(h)\psi^t - \psi^t}{h} &= \frac{1}{h}\Big[U(h)\Big(\int_0^t U(s)\psi\,ds\Big) - \int_0^t U(s)\psi\,ds\Big] = \frac{1}{h}\int_0^t U(h+s)\psi\,ds - \frac{1}{h}\int_0^t U(s)\psi\,ds\\ &= \frac{1}{h}\int_h^{t+h} U(s)\psi\,ds - \frac{1}{h}\int_0^t U(s)\psi\,ds = \frac{1}{h}\int_t^{t+h} U(s)\psi\,ds - \frac{1}{h}\int_0^h U(s)\psi\,ds\end{aligned}$$

Therefore, we find

$$\begin{aligned}\lim_{h\to 0}\frac{U(h)\psi^t - \psi^t}{h} &= \lim_{h\to 0}\Big(\frac{1}{h}\int_t^{t+h} U(s)\psi\,ds - \frac{1}{h}\int_0^h U(s)\psi\,ds\Big) = \lim_{h\to 0}\Big(U(t)\frac{\psi_h}{h} - \frac{\psi_h}{h}\Big)\\ &= U(t)\psi - \psi\end{aligned}$$

Hence, $s \mapsto U(s)\psi^t$ is differentiable, so $\psi^t \in \mathrm{dom}(H)$, with

$$H\psi^t = i\frac{d}{dt}U(t)\psi|_{t=0} = i(U(t)\psi - \psi) \tag{2.10}$$

This completes the proof of (1).
To prove that H is closed, let $(\psi_k)_{k\in\mathbb{N}}$ be a sequence in $\mathrm{dom}(H)$ with $\psi_k \to \psi$ and $H\psi_k \to \eta$ as $k \to \infty$ for some $\psi, \eta \in \mathcal{H}$. For fixed $h \neq 0$ with the continuity of $U(t)$ on $\mathcal{H}$ for all $t \in \mathbb{R}$ and the fundamental theorem of calculus:

$$\begin{aligned} i\frac{U(h)\psi - \psi}{h} &= i\lim_{k\to\infty} \frac{U(h)\psi_k - U(0)\psi_k}{h} = \lim_{k\to\infty} \frac{1}{h}\int_0^h i\Big(\frac{d}{ds}U(s)\psi_k\Big)\, ds \\ &= \lim_{k\to\infty} \frac{1}{h}\int_0^h U(s)H\psi_k\, ds = \frac{1}{h}\int_0^h U(s)\eta\, ds \xrightarrow{h\to 0} \eta \end{aligned}$$

where we used continuity of $s \mapsto U(s)H\psi_k$ on compact subsets of $\mathbb{R}$ to interchange the limit and the integral. Thus, $\psi \in \mathrm{dom}(H)$ and $H\psi = \eta$. □

Point (1) implies that H is a generator of the unitary group $(U(t))_{t\in\mathbb{R}}$ by Definition (2.3).
Thus, we have derived that every unitary group $(U(t))_{t\in\mathbb{R}}$ has at least one generator H which is given by (2.8) and every generator is a closed operator. The following property will play a fundamental role in the study of operators.

Definition 2.5. An operator $A : \mathrm{dom}(A) \to \mathcal{H}$ is called symmetric if $\langle \varphi, A\psi\rangle = \langle A\varphi, \psi\rangle$ holds for all $\varphi, \psi \in \mathrm{dom}(A)$.

Theorem 2.6. Let H be a generator of a unitary group $(U(t))_{t\in\mathbb{R}}$, then H is symmetric.

Proof. Let H be a generator and $\varphi, \psi \in \mathrm{dom}(H)$. Then, we compute

$$\begin{aligned} 0 = \frac{d}{dt}\langle \varphi, \psi\rangle &= \frac{d}{dt}\langle U(t)\varphi, U(t)\psi\rangle = \langle -iHU(t)\varphi, U(t)\psi\rangle + \langle U(t)\varphi, -iHU(t)\psi\rangle \\ &= i\langle U(t)H\varphi, U(t)\psi\rangle - i\langle U(t)\varphi, U(t)H\psi\rangle = i(\langle H\varphi, \psi\rangle - \langle \varphi, H\psi\rangle). \end{aligned}$$

Therefore, H is symmetric. □

Up to this point, we were able to obtain closedness and symmetry of H. However, as already mentioned above, the generator could possibly be unbounded and therefore hard to handle. Instead, we will continue to work with its resolvent operators which are bounded by definition. To define these, we need the following multiplication operator.

Definition 2.6. Let $V : \mathbb{R}^n \to \mathbb{C}$ be a continuous function and $D := \big\{f \in L^2(\mathbb{R}^n) \,|\, V \cdot f \in L^2(\mathbb{R}^n)\big\}$. We define the multiplication operator $T_V : D \to L^2(\mathbb{R}^n), (T_V f)(x) := V(x)f(x)$.

We will denote the multiplication operator T_V by V itself and give an explicit remark when we are talking about the function instead of the operator.
For example, we will use the multiplication operator $zI = z$ for the constant function $z \in \mathbb{C}$. The sum with another operator $A : \mathrm{dom}(A) \to \mathcal{H}$ is defined as $A + z : \mathrm{dom}(A) \to \mathcal{H}, (A + z)\varphi = A\varphi + z\varphi$. Trivially, the multiplication with a constant is commutating with A as long as the domains are sufficient.

Definition 2.7 (Resolvent)**.** Let $A : \mathrm{dom}(A) \to \mathcal{H}$ be a linear operator. The resolvent set of A is defined by

$$\rho(A) := \left\{ z \in \mathbb{C} \,|\, (z - A) : \mathrm{dom}(A) \to \mathcal{H} \text{ is a bijection and } (z - A)^{-1} \text{ is bounded} \right\}$$

and its compliment in $\mathbb{C}$ is the spectrum of A, $\sigma(A) := \mathrm{spec}(A) := \mathbb{C} \setminus \rho(A)$.
We refer to $R_z : \mathcal{H} \to \mathrm{dom}(A), R_z := (z - A)^{-1}$ as the resolvent operator for $z \in \rho(A)$.

Since the resolvent operator contains information about H itself, we will take a closer look at them now. In the following theorem we find an explicit expression of the resolvent operator $R_{i\lambda}$ of H for all $\lambda \in \mathbb{R} \setminus \{0\}$.

Theorem 2.7 (Resolvent identities)**.**

(1) For $\lambda, \mu \in \rho(H)$, we have

$$R_\lambda - R_\mu = (\mu - \lambda) R_\lambda R_\mu \tag{2.11}$$

and

$$R_\lambda R_\mu = R_\mu R_\lambda. \tag{2.12}$$

(2) a) If $\lambda > 0$, then $i\lambda \in \rho(H)$ and for $\psi \in \mathrm{dom}(H)$ we have

$$R_{i\lambda}\psi = -i \int_0^\infty e^{-\lambda t} U(t)\psi \, dt. \tag{2.13}$$

b) If $\lambda > 0$, then $-i\lambda \in \rho(H)$ and for $\psi \in \mathrm{dom}(H)$ we have

$$R_{-i\lambda}\psi = i \int_{-\infty}^0 e^{\lambda t} U(t)\psi \, dt. \tag{2.14}$$

Proof.

(1) By definition we have $I = R_\lambda(\lambda - H)$ on $\mathrm{dom}(H)$ and $I = (\lambda - H)R_\lambda$ on $\mathcal{H}$. Hence

$$\begin{aligned} R_\lambda - R_\mu &= R_\lambda(\mu - H)R_\mu - R_\lambda(\lambda - H)R_\mu = R_\lambda((\mu - H) - (\lambda - H))R_\mu \\ &= R_\lambda(\mu - \lambda)R_\mu = (\mu - \lambda)R_\lambda R_\mu \end{aligned}$$

since the multiplication with a constant $\mu - \lambda$ commutes with R_λ.

We use (2.11) by switching the constants to obtain the second identity:

$$R_\lambda R_\mu = \frac{1}{\mu - \lambda}(R_\lambda - R_\mu) = \frac{1}{\lambda - \mu}(R_\mu - R_\lambda) = R_\mu R_\lambda$$

(2) a) The Bochner integral is defined since $\lambda > 0$, $\|U(t)\| = 1$, so $\|U(t)\psi\| = \|\psi\|$ and the integrand is continuous.

Let $\tilde{R}_{i\lambda}$ denote the right hand side. For $h \neq 0$ and $\psi \in \mathcal{H}$ we have

$$\frac{U(h)\tilde{R}_{i\lambda}\psi - \tilde{R}_{i\lambda}\psi}{h} = -i\frac{1}{h}\int_0^\infty e^{-\lambda t}(U(t+h)\psi - U(t)\psi)\,dt$$

$$= -i\Big(-\frac{1}{h}\int_0^h e^{-\lambda(t-h)}U(t)\psi\,dt + \frac{1}{h}\int_0^\infty (e^{-\lambda(t-h)} - e^{-\lambda t})U(t)\psi\,dt\Big)$$

$$= ie^{\lambda h}\frac{1}{h}\int_0^h e^{-\lambda t}U(t)\psi\,dt + \frac{e^{\lambda h}-1}{h}(-i)\int_0^\infty e^{-\lambda t}U(t)\psi\,dt.$$

Hence, we may safely take the limit $h \to 0$ and obtain

$$\lim_{h\to 0}\frac{U(h)\tilde{R}_{i\lambda}\psi - \tilde{R}_{i\lambda}\psi}{h} = iU(0)\psi + \big(\lim_{h\to 0}\frac{e^{\lambda h}-1}{h}\big)\tilde{R}_{i\lambda}\psi = i\psi + \lambda\tilde{R}_{i\lambda}\psi.$$

Thus, $\tilde{R}_{i\lambda}\psi \in \mathrm{dom}(H)$ and $H\tilde{R}_{i\lambda}\psi = i(i\psi + \lambda\tilde{R}_{i\lambda}\psi) = -\psi + i\lambda\tilde{R}_{i\lambda}\psi$ and for $\psi \in \mathcal{H}$:

$$(i\lambda - H)\tilde{R}_{i\lambda}\psi = \psi$$

H is closed, so we can interchange it with the integral. For $\psi \in \mathrm{dom}(H)$:

$$H\tilde{R}_{i\lambda}\psi = -iH\int_0^\infty e^{-\lambda t}U(t)\psi\,dt = -i\int_0^\infty e^{-\lambda t}HU(t)\psi\,dt = -i\int_0^\infty e^{-\lambda t}U(t)H\psi\,dt$$

$$= \tilde{R}_{i\lambda}H\psi$$

H and $\tilde{R}_{i\lambda}$ commutate, so

$$\tilde{R}_{i\lambda}(i\lambda - H)\psi = \psi.$$

Hence $i\lambda - H : \mathrm{dom}(H) \to \mathcal{H}$ is bijective and $\tilde{R}_{i\lambda} = (i\lambda - H)^{-1} = R_{i\lambda}$. We have

$$\left\|\int_0^\infty e^{-\lambda t}U(t)\psi\,dt\right\| \leq \int_0^\infty e^{-\lambda t}\,\|U(t)\psi\|\,dt = \|\psi\|\int_0^\infty e^{-\lambda t}dt = \frac{1}{\lambda}\psi.$$

This results in an upper bound for the norm of the resolvent operator:

$$\|R_{i\lambda}\| = \sup_{\psi\in\mathcal{H}}\frac{\left\|\int_0^\infty e^{-\lambda t}U(t)\psi\,dt\right\|}{\|\psi\|} \leq \frac{1}{\lambda}$$

Thus, $i\lambda - H$ is bijective with a bounded inverse, so $i\lambda \in \rho(H)$.

b) This case follows analogously with switched signs, we will rewrite the most important parts. The integral is defined since $\lambda > 0$.

Let $\tilde{R}_{-i\lambda}$ denote the right hand side. For $h \neq 0$ and $\psi \in \mathcal{H}$ we have

$$\frac{U(h)\tilde{R}_{-i\lambda}\psi - \tilde{R}_{-i\lambda}\psi}{h} = i\frac{1}{h}\int_{-\infty}^0 e^{\lambda t}(U(t+h)\psi - U(t)\psi)\,dt$$

$$= i\Big(\frac{1}{h}\int_0^h e^{\lambda(t-h)}U(t)\psi\,dt + \frac{1}{h}\int_{-\infty}^0 (e^{\lambda(t-h)} - e^{\lambda t})U(t)\psi\,dt\Big)$$

$$= ie^{-\lambda h}\frac{1}{h}\int_0^h e^{\lambda t}U(t)\psi\,dt + \frac{e^{-\lambda h}-1}{h}\,i\int_{-\infty}^0 e^{\lambda t}U(t)\psi\,dt.$$

Hence,

$$\lim_{h\to 0}\frac{U(h)\tilde{R}_{-i\lambda}\psi-\tilde{R}_{-i\lambda}\psi}{h}=iU(0)\psi+\big(\lim_{h\to 0}\frac{e^{-\lambda h}-1}{h}\big)\tilde{R}_{-i\lambda}\psi=i\psi-\lambda\tilde{R}_{-i\lambda}\psi.$$

Thus, $\tilde{R}_{-i\lambda}\psi\in\mathrm{dom}(H)$ and $H\tilde{R}_{-i\lambda}\psi=i(i\psi-\lambda\tilde{R}_{-i\lambda}\psi)=-\psi-i\lambda\tilde{R}_{-i\lambda}\psi$ and for $\psi\in\mathcal{H}$:

$$(-i\lambda-H)\tilde{R}_{-i\lambda}\psi=\psi$$

For $\psi\in\mathrm{dom}(H)$:

$$H\tilde{R}_{-i\lambda}\psi=iH\int_{-\infty}^{0}e^{\lambda t}U(t)\psi\,dt=i\int_{-\infty}^{0}e^{\lambda t}HU(t)\psi\,dt=i\int_{-\infty}^{0}e^{\lambda t}U(t)H\psi\,dt=\tilde{R}_{-i\lambda}H\psi$$

H and $\tilde{R}_{-i\lambda}$ commutate, so

$$\tilde{R}_{-i\lambda}(-i\lambda-H)\psi=\psi.$$

Hence $-i\lambda-H:\mathrm{dom}(H)\to\mathcal{H}$ is bijective and $\tilde{R}_{-i\lambda}=(-i\lambda-H)^{-1}=R_{-i\lambda}$. We have

$$\left\|\int_{-\infty}^{0}e^{\lambda t}U(t)\psi\,dt\right\|\leq\int_{-\infty}^{0}e^{\lambda t}\left\|U(t)\psi\right\|dt=\|\psi\|\int_{-\infty}^{0}e^{\lambda t}dt=\frac{1}{\lambda}\psi.$$

This results in an upper bound for the norm of the resolvent operator:

$$\|R_{-i\lambda}\|=\sup_{\psi\in\mathcal{H}}\frac{\left\|\int_{-\infty}^{0}e^{\lambda t}U(t)\psi\,dt\right\|}{\|\psi\|}\leq\frac{1}{\lambda}$$

Thus, $-i\lambda-H$ is bijective with a bounded inverse, so $-i\lambda\in\rho(H)$. □

Theorem 2.8. Let $(U(t))_{t\in\mathbb{R}}$ be a unitary group on $\mathcal{H}$, then it has a densely defined, closed generator H that satisfies

$$\pm i(0,\infty)\subseteq\rho(H)\quad\text{and}\quad\|R_{i\lambda}\|\leq\frac{1}{|\lambda|}\text{ for }\lambda\in\mathbb{R}\setminus\{0\}.\tag{2.15}$$

Proof. By Theorem (2.5), there is a densely defined, closed generator H of $(U(t))_{t\in\mathbb{R}}$, for which we have obtained $\pm i(0,\infty)\subseteq\rho(H)$ and the resolvent identities (2.13) and (2.14) in Theorem (2.7). In the above proof, we found that for $\lambda\neq 0$: $\|R_{i\lambda}\|\leq\dfrac{1}{|\lambda|}$. □

With this Theorem, we expanded our knowledge about the generator H even further: We found that the potentially unbounded operator H is closed, symmetric and its resolvent satisfies the properties (2.15).
Now, we want to use the topological structure of a Hilbert space to filter out the information about H that the resolvent operator holds. For this, we will focus on abstract operator theory in the next chapter.

3 Operator Theory

We give a short overview of what will be covered in this section. In the first part, we will develop tools which we will use in the second part to understand the properties of operators on a Hilbert space $\mathcal{H}$. Then, we apply the found results to the generator H.

3.1 Closed operators, resolvent and spectrum

We start on a more abstract setting in order to extend the above discussion. Let $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ be a general Hilbert space. We denote the space of bounded and linear operators mapping from $\mathcal{H}$ into itself as $\mathrm{BL}(\mathcal{H})$. First, let us state a well known lemma which we will use along the way to find the bounded inverse of operators.

Lemma 3.1 (Neumann)**.** Let $A \in \mathrm{BL}(\mathcal{H})$ with $\|A\| < 1$, then the operator $I - A$ is invertible and

$$(I-A)^{-1} = \sum_{k=0}^{\infty} A^k \quad \text{with} \quad \left\|(I-A)^{-1}\right\| \leq \frac{1}{1-\|A\|} \tag{3.1}$$

where the convergence is to be understood with respect to the operator norm.

Proof. [2, Sec. 2.4, Eq. (2.90)] □

Remember the definition (2.7) of the resolvent set of an operator. The complex numbers contained in this set each give a corresponding resolvent operator of H. Using the Neumann lemma, we can show that the resolvent set is open with respect to the standard topology on $\mathbb{C}$.

Theorem 3.2. $\rho(A)$ is open and $\sigma(A)$ is closed.

Proof. Let $z_0 \in \rho(A)$ and $z \in \mathbb{C}$ such that $|z - z_0| < \frac{1}{\|R_A(z_0)\|}$. Then

$$z - A = z_0 - A + (z - z_0) = (1 + (z - z_0)R_A(z_0))(z_0 - A) \tag{3.2}$$

By Lemma (3.1) the operator $1 + (z - z_0)R_A(z_0)$ is invertible with bounded inverse since

$$\|(z - z_0)R_A(z_0)\| = |z - z_0| \, \|R_A(z_0)\| < 1$$

Hence, $z - A$ is invertible and

$$(z-A)^{-1} = \big((1 + (z - z_0)R_A(z_0))(z_0 - A)\big)^{-1} = (z_0 - A)^{-1}(1 + (z - z_0)R_A(z_0))^{-1}$$

is bounded. Therefore, $\{z \in \mathbb{C} \,|\, |z - z_0| < \frac{1}{\|R_A(z_0)\|}\} \subseteq \rho(A)$, so $\rho(A)$ is open and its compliment $\sigma(A)$ is closed. □

Another tool we will need is the following connection between two operators.

Definition 3.1. Let A, B be linear operators on $\mathcal{H}$. If $\Gamma(A) \subseteq \Gamma(B)$ and $B\varphi = A\varphi$ for all $\varphi \in \mathrm{dom}(A)$, then B is called an extension of A and we write $A \subseteq B$.
A linear operator A is called closable if it has a closed extension. Then we refer to the smallest closed extension, i.e., the one with the smallest domain, as the closure of A and denote it by $\overline{A}$.

This helps us to understand more about a closed operator.

Theorem 3.3. Let $A : \mathrm{dom}(A) \to \mathcal{H}$ be a linear operator. Then, the following statements are equivalent:

(1) A is closable.

(2) $\overline{\Gamma(A)}$ is the graph of a linear operator.

(3) If $(\psi_n)_{n\in\mathbb{N}}$ is a sequence in $\mathrm{dom}(A)$ with $\psi_n \to 0$ and $A\psi_n \to \varphi$ as $n \to \infty$ for some $\varphi \in \mathcal{H}$, then $\varphi = 0$.

Proof.

- (1) $\implies$ (3): Let $A \subseteq B$ for some closed operator B. Consider a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $\mathrm{dom}(A)$ with $\psi_n \to 0$ and $A\psi_n \to \varphi \in \mathcal{H}$ as $n \to \infty$. As B is a closed extension of A, we have $B\psi_n \to \varphi$ and since B is closed, it follows that $\varphi = B \cdot \big(\lim_{n\to\infty} \psi_n\big) = 0$.

- (3) $\implies$ (2): We define the map $B : \mathrm{dom}(B) \to \mathcal{H}$ by $B\psi = y$ for $(\psi, \varphi) \in \overline{\Gamma(A)}$, consequently $\mathrm{dom}(B) := \big\{\psi \in \mathcal{H} \,|\, \exists \varphi \in \mathcal{H} : (\psi, \varphi) \in \overline{\Gamma(A)}\big\}$. It remains to prove that B is well-defined and linear. Consider $(\psi, \varphi_1), (\psi, \varphi_2) \in \overline{\Gamma(A)}$. The closed graph is a linear subspace, so $(\psi, \varphi_1 - \varphi_2) \in \Gamma(A)$. Thus, there exists a sequence $(\psi_n, A\psi_n)_{n\in\mathbb{N}}$ in $\overline{\Gamma(A)}$ with $\psi_n \to 0$ and $A\psi_n \to \varphi_1 - \varphi_2 \in \mathcal{H}$ as $n \to \infty$, so by (3) $\varphi_1 - \varphi_2 = 0 \implies \varphi_1 = \varphi_2$. Now let $(\psi_1, \varphi_1), (\psi_2, \varphi_2) \in \overline{\Gamma(A)}$ for some $\psi_1, \psi_2 \in \mathrm{dom}(B)$ and $\alpha, \beta \in \mathbb{R}$. Again, since the closed graph is a linear subspace, $(\alpha\psi_1 + \beta\psi_2, \alpha\varphi_1 + \beta\varphi_2) \in \overline{\Gamma(A)}$, so $B(\alpha\psi_1 - \beta\psi_2) = \alpha\varphi_1 + \beta\varphi_2$, therefore B is linear.

  We get $\mathrm{dom}(B) \supseteq \mathrm{dom}(A)$ and $\Gamma(B) = \overline{\Gamma(A)}$. Notice, that B is in particular the closure of A. Hence, every closable operator has indeed a closure.

- (2) $\implies$ (1): By assumption, there exists a linear operator B with $\Gamma(B) = \overline{\Gamma(A)}$. Hence, B is closed and $A \subseteq B$. $\square$

3.2 Symmetric and self-adjoint operators

Now we go back to the more specific setting of Section 2. Let $A : \mathrm{dom}(A) \subseteq \mathcal{H} \to \mathcal{H}$ be a densely defined linear operator. Note that such an operator could satisfy the basic requirements to be a generator as in Definition (2.3).

Definition 3.2. The adjoint of A is the unique operator $A^* : \mathrm{dom}(A^*) \to \mathcal{H}$, defined by

(1) $\mathrm{dom}(A^*) := \big\{\psi \in \mathcal{H} \,|\, \exists \eta \in \mathcal{H} : \langle \psi, A\varphi \rangle = \langle \eta, \varphi \rangle \, \forall \varphi \in \mathrm{dom}(A)\big\}$

(2) $A^*\psi = \eta$ from above

In order to check that the adjoint operator is well-defined for such a densely defined operator, we consider $\eta, \tilde{\eta} \in \mathcal{H}$ such that $\langle \eta, \varphi \rangle = \langle \tilde{\eta}, \varphi \rangle$ for all $\varphi \in \mathrm{dom}(A)$, then $\langle \eta - \tilde{\eta}, \psi \rangle = 0$. Since $\mathrm{dom}(A)$ is dense in $\mathcal{H}$, we get $\forall \psi \in \mathcal{H} : \langle \eta - \tilde{\eta}, \psi \rangle = 0$, so $\eta = \tilde{\eta}$ is unique. Similarly, $A^{**} = (A^*)^*$ is well-defined if and only if A^* is densely defined. By definition (3.1), a symmetric operator A satisfies $A \subseteq A^*$.

Notice that we have already seen the symmetry requirement on H in Theorem (2.6). However, it turns out that symmetry alone is not the strongest property of a generator and not enough for just any densely defined operator to be a generator of a unitary group. We rather need the following.

Definition 3.3. A is called self-adjoint if $A = A^*$, i.e. A is symmetric and $\mathrm{dom}(A) = \mathrm{dom}(A^*)$.

Lemma 3.4. If $A \subseteq B$, then $B^* \subseteq A^*$.

Proof. For all $\varphi \in \mathrm{dom}(A) \subseteq \mathrm{dom}(B) : A\varphi = B\varphi$. Let $\psi \in \mathrm{dom}(B^*)$ with $B^*\psi = \eta$ for some $\eta \in \mathcal{H}$, then especially for all $\varphi \in \mathrm{dom}(A)$, $\langle \psi, A\varphi \rangle = \langle \psi, B\varphi \rangle = \langle \eta, \varphi \rangle$, so $\psi \in \mathrm{dom}(A^*)$ with $A^*\psi = \eta = B^*\psi$, so A^* is an extension of B^*. $\square$

Theorem 3.5.

(1) A^* is closed.

(2) If A is closable, then $(\overline{A})^* = A^*$.

(3) If $\mathrm{dom}(A^*)$ is dense in $\mathcal{H}$, then A is closable.

Proof.

(1) Let $(\psi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathrm{dom}(A^*)$ with $\psi_n \to \psi$ and $A^*\psi_n \to \eta$ as $n \to \infty$ for some $\psi, \eta \in \mathcal{H}$. Then for all $\varphi \in \mathrm{dom}(A)$: $\langle \psi, A\varphi \rangle = \lim\limits_{n\to\infty} \langle \psi_n, A\varphi \rangle = \lim\limits_{n\to\infty} \langle A^*\psi_n, \varphi \rangle = \langle \eta, \varphi \rangle$. Therefore, $\psi \in \mathrm{dom}(A^*)$ and $A^*\psi = \eta$.

(2) If A is closable, we have $A \subseteq \overline{A}$ and using Lemma (3.4) we get $\overline{A}^* \subseteq A^*$. It remains to prove $\mathrm{dom}(A^*) \subseteq \mathrm{dom}(\overline{A}^*)$. Let $\psi \in \mathrm{dom}(A^*)$ and $\varphi \in \mathrm{dom}(\overline{A})$. Then there is a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $\mathrm{dom}(A)$ with $\varphi_n \to \varphi$ and $A\varphi_n \to \overline{A}\varphi$ as $n \to \infty$. We have $\left\langle \psi, \overline{A}\varphi \right\rangle = \lim_{n\to\infty} \langle \psi, A\varphi_n \rangle = \lim_{n\to\infty} \langle A^*\psi, \varphi_n \rangle = \langle A^*\psi, \varphi \rangle$, since $\psi \in \mathrm{dom}(A^*)$. Thus, for all $\varphi \in \mathrm{dom}(\overline{A}) : \left\langle \psi, \overline{A}\varphi \right\rangle = \langle A^*\psi, \varphi \rangle \implies \psi \in \mathrm{dom}(\overline{A}^*)$.

(3) Let $(\psi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathrm{dom}(A)$ with $\psi_n \to 0$ and $A\psi_n \to \eta \in \mathcal{H}$ as $n \to \infty$. Then for all $\varphi \in \mathrm{dom}(A^*)$:

$$\langle \varphi, \eta \rangle = \lim_{n\to\infty} \langle \varphi, A\psi_n \rangle = \lim_{n\to\infty} \langle A^*\varphi, \psi_n \rangle = \langle A^*\varphi, 0 \rangle = 0$$

If $\mathrm{dom}(A^*)$ is dense, we get $\eta = 0$. By Theorem (3.3) (3), A is closable. $\square$

In particular, every densely defined symmetric operator A is closable, since $\mathrm{dom}(A) \subseteq \mathrm{dom}(A^*)$ is dense in $\mathcal{H}$. Furthermore, this implies that every self-adjoint operator is closed.

Theorem 3.6. $\ker(A^*) = \mathrm{ran}(A)^\perp$. Thus, $\mathrm{ran}(A)^\perp \subseteq \mathrm{dom}(A^*)$ and $\ker(A^*) = \{0\}$ if and only if $\overline{\mathrm{ran}(A)} = \mathcal{H}$.

Proof. We have

$$\psi \in \ker(A^*) \iff A^*\psi = 0 \iff \forall \varphi \in \mathrm{dom}(A) : \langle A^*\psi, \varphi \rangle = \langle \psi, A\varphi \rangle = 0 \iff \psi \in \mathrm{ran}(A)^\perp.$$

This proves $\ker(A^*) = \mathrm{ran}(A)^\perp$ and with $\ker(A^*) \subseteq \mathrm{dom}(A^*)$ we get $\mathrm{ran}(A)^\perp \subseteq \mathrm{dom}(A^*)$. Since $\mathcal{H} = \overline{\mathrm{ran}(A)} \oplus \overline{\mathrm{ran}(A)}^\perp = \overline{\mathrm{ran}(A)} \oplus \mathrm{ran}(A)^\perp = \overline{\mathrm{ran}(A)} \oplus \ker(A^*)$, the second statement follows. $\square$

Example 3.1. The adjoint operator of $A + z$ is $A^* + \overline{z} : \mathrm{dom}(A^*) \to \mathcal{H}$ where $\overline{z}$ denotes the complex conjugate of z. Indeed, for all $\psi \in \mathrm{dom}(A^*), \varphi \in \mathrm{dom}(A)$:

$$\langle \psi, (A + z)\varphi \rangle = \langle \psi, A\varphi \rangle + z \langle \psi, \varphi \rangle = \langle A^*\psi, \varphi \rangle + \langle \overline{z}\psi, \varphi \rangle = \langle (A^* + \overline{z})\psi, \varphi \rangle$$

Before we can formulate the main result of this chapter, there is one more identity we will use multiple times.

Lemma 3.7. Let A be symmetric. For all $\lambda, \mu \in \mathbb{R}$ and $\varphi \in \operatorname{dom}(A)$:

$$\|(A - \lambda - i\mu)\varphi\|^2 = \|(A - \lambda)\varphi\|^2 + \mu^2 \|\varphi\|^2$$

Proof. We have

$$\begin{aligned} \|(A - \lambda - i\mu)\varphi\|^2 &= \langle (A - \lambda - i\mu)\varphi, (A - \lambda - i\mu)\varphi \rangle \\ &= \|(A - \lambda)\varphi\|^2 + \mu^2 \|\varphi\|^2 + 2\operatorname{Re}(i \langle (A - \lambda)\varphi, \mu\varphi \rangle) = \|(A - \lambda)\varphi\|^2 + \mu^2 \|\varphi\|^2 \end{aligned}$$

where the last term vanishes since A and therefore $A - \lambda$ is symmetric, so

$$\langle (A - \lambda)\varphi, \mu\varphi \rangle = \langle \mu\varphi, (A - \lambda)\varphi \rangle \in \mathbb{R}.$$

In particular, $\|(A - \lambda - i\mu)\varphi\|^2 \geq |\mu|^2 \|\varphi\|^2$. □

Now we are in a position to connect the properties of densely definedness and closedness, which also apply to operators on Banach spaces, with the property of self-adjointness in Hilbert spaces. The following Theorem can be found in [4, Sec. VIII, Thm VIII.3]. It is essential to view the characterisation of generators (2.15) in the explicit setting of a Hilbert space. We will also use the criteria later to study common examples of Hamiltonian operators in quantum physics.

Theorem 3.8 (Criteria for self-adjointness).
Let $A : \operatorname{dom}(A) \to \mathcal{H}$ be a densely defined symmetric operator. Then the following assertions are equivalent:

(1) A is self-adjoint

(2) A is closed and $\ker(A^* \pm i\mu) = \{0\}$ holds for both signs and some $\mu \in \mathbb{R} \setminus \{0\}$

(3) $\operatorname{ran}(A \pm i\mu) = \mathcal{H}$ holds for both signs and some $\mu \in \mathbb{R} \setminus \{0\}$

Proof.

- (1) $\implies$ (2): $A = A^*$ is closed by Theorem (3.5). Let $\varphi \in \ker(A^* - i\mu)$ and $\mu \neq 0$ arbitrary, then $A\varphi = A^*\varphi = i\mu\varphi$ and

  $$i\mu \langle \varphi, \varphi \rangle = \langle \varphi, i\mu\varphi \rangle = \langle \varphi, A\varphi \rangle = \langle A^*\varphi, \varphi \rangle = -i\mu \langle \varphi, \varphi \rangle \implies \|\varphi\| = 0 \implies \varphi = 0.$$

  Hence, $\ker(A^* - i\mu) = \{0\}$.

- (2) $\implies$ (3): By Theorem (3.6) and Example (3.1) we have $\ker(A^* \pm i\mu) = \{0\} \iff \operatorname{ran}(A \mp i\mu)^\perp$ is dense in $\mathcal{H}$, so it remains to prove that $\operatorname{ran}(A \pm i\mu)$ is closed.

  Let $\eta \in \mathcal{H}$. Since $\operatorname{ran}(A - i\mu)$ is dense, there is a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $\operatorname{dom}(A)$ such that $(A - i\mu)\varphi_n \xrightarrow{n\to\infty} \eta$. Then $(A - i\mu)\varphi_n$ is Cauchy and by Lemma (3.7) with $\lambda = 0$, φ_n is Cauchy. By the completeness of $\mathcal{H}$, there exists some $\psi \in \mathcal{H}$ such that $\varphi_n \xrightarrow{n\to\infty} \psi$.

  We get $(A - i\mu)\varphi_n = A\varphi_n - i\mu\varphi_n \to \eta$, so $A\varphi_n \to \eta + i\mu\psi$ as $n \to \infty$. A is closed, therefore $\psi \in \operatorname{dom}(A)$ and $A\psi = \eta + i\mu\psi \implies (A - i\mu)\psi = \eta \in \operatorname{ran}(A - i\mu)$. Hence, $\operatorname{ran}(A - i\mu) = \mathcal{H}$.

  Analogously for $\operatorname{ran}(A + i\mu)$ with $\ker(A^* - i\mu)$.

- (3) $\implies$ (1): Let $\psi \in \mathrm{dom}(A^*)$. There exists a $\varphi \in \mathrm{dom}(A)$ such that $(A^* - i\mu)\psi = (A - i\mu)\varphi$. Since A is symmetric, we have $A \subseteq A^*$, so $(A^* - i\mu)(\psi - \varphi) = 0$. For all $\eta \in \mathrm{dom}(A)$:
$$\langle \psi - \varphi, (A + i\mu)\eta \rangle = \langle (A^* - i\mu)(\psi - \varphi), \eta \rangle = 0$$
We have $\{(A+i\mu)\eta \,|\, \eta \in \mathrm{dom}(A)\} = \mathcal{H}$, so $\psi = \varphi \in \mathrm{dom}(A) \implies A^* \subseteq A$, so $A = A^*$. $\square$

We define the two halfspaces $\mathbb{C}_+ := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) > 0\}$ and $\mathbb{C}_- := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) < 0\}$.

Theorem 3.9. Let A be symmetric.

(1) If $\mathrm{ran}(A - z_+) = \mathcal{H}$ for one $z_+ \in \mathbb{C}_+$, then $\mathbb{C}_+ \subseteq \rho(A)$.

(2) If $\mathrm{ran}(A + z_-) = \mathcal{H}$ for one $z_- \in \mathbb{C}_-$, then $\mathbb{C}_- \subseteq \rho(A)$.

Proof. We prove (1), part (2) works analogously. By Lemma (3.7), $\|(A - z_+)\varphi\| \geq |\mathrm{Im}(z_+)| \, \|\varphi\|$. If $(A - z_+)\varphi = 0$, then $\|\varphi\|^2 = 0 \implies \varphi = 0$. Hence , $A - z_+$ is injective. By assumption it is onto, so $(A - z_+)^{-1} : \mathcal{H} \to \mathrm{dom}(A)$ exists.
Inserting $\varphi = (A - z_+)^{-1}\psi$ into the inequality above gives $\left\|(A - z_+)^{-1}\psi\right\| \leq \dfrac{\|\psi\|}{|\mathrm{Im}(z_+)|}$.
Hence, $(A - z_+)$ is bounded. In particular, $z \in \rho(A)$ and $\|(A - z_+)\| \leq \dfrac{1}{|\mathrm{Im}(z_+)|}$.
By Theorem (3.2) $B(z_+, \left\|(A - z_+)^{-1}\right\|^{-1}) \subseteq B(z_+, |\mathrm{Im}(z_+)|) \subseteq \rho(A)$.
Iterating this argument for some z'_+ in this neighbourhood gives $\mathbb{C}_+ \in \rho(A)$. $\square$

With this Theorem we get one more criterion for self-adjointness, [4, Thm VI.8].

Lemma 3.10. Let A be symmetric. A is self-adjoint if and only if $\sigma(A) \subseteq \mathbb{R}$.

Proof. Let A be self-adjoint, then by (3.8) (3) we have $\mathrm{ran}(A - z_\pm) = \mathcal{H}$ for some $z_+ \in \mathbb{C}_+$ and $z_- \in \mathbb{C}_-$. By Theorem (3.9) we have $\mathbb{C}_+ \subseteq \rho(A)$ and $\mathbb{C}_- \subseteq \rho(A)$. Thus $\sigma(A) = \mathbb{C} \setminus \rho(A) \subseteq \mathbb{R}$.

Let $\sigma(A) \subseteq \mathbb{R}$. This is shown in the proof of Theorem (3.8) (3) $\implies$ (1) with an arbitrary $i\mu \in \rho(A), \mu \neq 0$. $\square$

Up to this point, we found multiple properties of a generator H of a unitary group $(U(t))_{t\in\mathbb{R}}$ in section 2. Namely, H is densely defined, closed and by Theorem (2.8) we have $\pm i \in \rho(H)$. Theorem (3.9) implies $\mathbb{C}_+ \cup \mathbb{C}_- \subseteq \rho(H)$. Equivalently $\sigma(H) \subseteq \mathbb{R}$, therefore the generator H is self-adjoint. Conversely, we want to see that every such H is the generator of a unitary group in the next section.

4 Hille-Yosida Theorem

In the following, we can use the theory we just covered to derive the Hille-Yosida Theorem in its full form for Hilbert spaces.

Theorem 4.1 (Hille-Yosida Theorem)**.** A densely defined, closed linear operator H on $\mathcal{H}$ is the generator of a unitary group $(U(t))_{t\in\mathbb{R}}$ if and only if

$$\pm i(0, \infty) \subseteq \rho(H) \quad \text{and} \quad \|R_{i\lambda}\| \leq \frac{1}{|\lambda|} \text{ for } \lambda \in \mathbb{R} \setminus \{0\}. \tag{4.1}$$

In the more general setting, when we consider the differential equation on just a Banach space X instead of a Hilbert space $\mathcal{H}$, this result takes on a similar form. For strongly continuous groups $U(t)$ on X satisfying $\|U(t)\| \leq e^{\omega|t|}$ for some $\omega \in \mathbb{R}_+$, the generator satisfies $\pm i(\omega, \infty) \in \rho(H)$ and $\|R_{i\lambda}\| \leq \frac{1}{|\lambda|-\omega}$. In order to get the desired unitarity of the group, we need $\omega = 0$, then $\pm i(0, \infty) \in \rho(H)$, so H must be self-adjoint. For further explanation, see [3, Sec. 7.4.2].
The key result of this theorem are the necessary and sufficient requirements on an operator in order to be the generator of a unitary group.
Before we prove this Theorem, we want to translate this into the physical setting. Given the self-adjoint Hamiltonian operator of a quantum system and an initial condition $\psi \in \mathcal{H}$, we obtain a solution $\psi(t) = U(t)\psi$ for all t by constructing a unitary group $(U(t))_{t\in\mathbb{R}}$ with generator H. This is done by evolving ψ forwards in time by using $i(0, \infty) \subseteq \rho(H)$ and backwards in time with $-i(0, \infty) \subseteq \rho(H)$. For a detailed discussion also compare [3, Sec. 7.4, Thm.4].
Before we begin with the proof, we observe that H and the resolvent operator R_λ are interchangeable for $\lambda \in \rho(H)$.

Lemma 4.2. Let $H : \mathrm{dom}(H) \to \mathcal{H}$ be linear. For $\lambda \in \rho(H)$ the operator $HR_\lambda = \lambda R_\lambda - I$ is an extension of $R_\lambda H$.

Proof. By definition, $\mathrm{dom}(R_\lambda H) = \mathrm{dom}(H) \subseteq \mathcal{H} = \mathrm{dom}(HR_\lambda)$ and $(\lambda - H)R_\lambda\psi = \psi$ for all $\psi \in \mathcal{H}$. On $\mathrm{dom}(H)$ we have $R_\lambda H = R_\lambda(\lambda - \lambda + H) = \lambda R_\lambda - R_\lambda(\lambda - H) = \lambda R_\lambda - I = \lambda R_\lambda - (\lambda - H)R_\lambda = HR_\lambda$. □

Now let us prove the Hille-Yosida Theorem.

Proof. For only if: We have constructed a generator H for an arbitrary unitary group $(U(t))_{t\in\mathbb{R}}$ that satisfies (4.1) in Theorem (2.8).
For if: Assume that (4.1) holds. The goal is to build a unitary group with H as its generator. Since this will be a fairly long proof, we give a structural outline to follow:

(1) First we "approximate" the possibly unbounded operator H with bounded operators $H_\lambda, \lambda \in \mathbb{R}$. Bounded and therefore continuous operators are always easier to handle.

(2) For the bounded operator H_λ there is an obvious candidate for a well-defined $U_\lambda(t)$ that might satisfy similar requirements for a unitary group with generator H_λ.

(3) Taking the limit $\lambda \to \pm\infty$, determined by the sign of t, we find a well-defined group $(U(t))_{t\in\mathbb{R}}$.

(4) Lastly, we can prove that $(U(t))_{t\in\mathbb{R}}$ is a unitary group with generator H.

(1) First, fix $\lambda \neq 0$ and define $H_\lambda := -i\lambda - \lambda^2 R_{i\lambda} = i\lambda(-(i\lambda - H) + i\lambda)(i\lambda - H)^{-1} = i\lambda HR_{i\lambda}$ on $\mathcal{H}$. We first claim for $\psi \in \mathrm{dom}(H)$:

$$H_\lambda\psi \to H\psi \text{ as } \lambda \to \pm\infty \tag{4.2}$$

Indeed, in the proof of the resolvent identities (5.7) we found $i\lambda R_{i\lambda}\psi - \psi = HR_{i\lambda}\psi = R_{i\lambda}H\psi$, so we have $\|i\lambda R_{i\lambda}\psi - \psi\| \leq \|R_{i\lambda}\| \, \|H\psi\| \leq \frac{1}{|\lambda|} \|H\psi\| \to 0$ as $\lambda \to \pm\infty$ and therefore $i\lambda R_{i\lambda}\psi \to \psi$ for $\psi \in \mathrm{dom}(H)$. But since $\|i\lambda R_{i\lambda}\| \leq 1$ and $\mathrm{dom}(H)$ is dense, we deduce

$$i\lambda R_{i\lambda}\psi \to \psi \text{ as } \lambda \to \pm\infty \text{ for all } \psi \in \mathcal{H}. \tag{4.3}$$

Now if $\psi \in \mathrm{dom}(H)$, then

$$H_\lambda \psi = i\lambda H R_{i\lambda}\psi = i\lambda R_{i\lambda} H\psi. \tag{4.4}$$

Combining this with (4.3), the claim (4.2) follows.
(2) For $t \in \mathbb{R}$ define

$$U_\lambda(t) := e^{-iH_\lambda t} = e^{-\lambda t} e^{i\lambda^2 t R_{i\lambda}} := e^{-\lambda t}\sum_{k=0}^{\infty} \frac{(i\lambda^2 t)^k}{k!} R_{i\lambda}^k.$$

$U_\lambda(t)$ is linear for all $\lambda, t \in \mathbb{R}$ since $R_{i\lambda}$ is linear. Using $\|R_{i\lambda}\| \le \frac{1}{|\lambda|}$, we see that the sum is a Cauchy sequence. In fact, for $N, M \in \mathbb{N}, N > M$:

$$\left\|\sum_{k=0}^{N} \frac{(i\lambda^2 t)^k}{k!} R_{i\lambda}^k - \sum_{k=0}^{M} \frac{(i\lambda^2 t)^k}{k!} R_{i\lambda}^k\right\| = \left\|\sum_{k=M+1}^{N} \frac{(i\lambda^2 t)^k}{k!} R_{i\lambda}^k\right\| \le \sum_{k=M+1}^{N} \frac{|\lambda|^{2k}\,|t|^k}{k!}\,\|R_{i\lambda}\|^k$$

$$\le \sum_{k=M+1}^{N} \frac{|\lambda|^{k}\,|t|^k}{k!} \xrightarrow{N,M\to\infty} 0$$

Therefore, $U_\lambda(t)$ is well-defined on all of $\mathcal{H}$. Now, we study properties of the group $(U_\lambda(t))_{t\in\mathbb{R}}$ in the hope of them being similar to the ones of a unitary group.

$$\|U_\lambda(t)\| \le e^{-\lambda t}\sum_{k=0}^{\infty} \frac{|\lambda|^{2k}\,|t|^k}{k!}\,\|R_{i\lambda}\|^k \le e^{-\lambda t}\sum_{k=0}^{\infty} \frac{|\lambda|^{k}\,|t|^k}{k!} = e^{-\lambda t} e^{|\lambda||t|},$$

so $U_\lambda(t)$ is bounded for all $\lambda \in \mathbb{R}\setminus\{0\}$ and $t \in \mathbb{R}$. In particular, if $\mathrm{sign}(\lambda) = \mathrm{sign}(t)$ we get $\|U_\lambda(t)\| \le 1$. Furthermore, for all $s, t \in \mathbb{R}$:

$$U_\lambda(t+s) = e^{-\lambda(t+s)} e^{\lambda^2 (t+s) R_{i\lambda}} = e^{-\lambda t} e^{-\lambda s}\sum_{k=0}^{\infty} \frac{(i\lambda^2)^k}{k!}(t+s)^k R_{i\lambda}^k$$

$$= e^{-\lambda t} e^{-\lambda s}\sum_{k=0}^{\infty}\sum_{n+m=k} \frac{(i\lambda^2)^k}{k!}\binom{k}{n} t^n s^m R_{i\lambda}^k = e^{-\lambda t} e^{-\lambda s}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{(i\lambda^2 t)^n}{n!} R_{i\lambda}^n \frac{(i\lambda^2 s)^m}{m!} R_{i\lambda}^m$$

$$= \big(e^{-\lambda t}\sum_{n=0}^{\infty} \frac{(i\lambda^2 t)^n}{n!} R_{i\lambda}^n\big)\big(e^{-\lambda s}\sum_{m=0}^{\infty} \frac{(i\lambda^2 s)^m}{m!} R_{i\lambda}^m\big) = U_\lambda(t)U_\lambda(s)$$

where we interchanged the order of summation because $U_\lambda(t+s)$ converges in operator norm. The group is strongly continuous since

$$t \mapsto e^{-\lambda t}\sum_{k=0}^{\infty} \frac{(i\lambda^2 t)^k}{k!} R_{i\lambda}^k \psi$$

is well-defined and continuous in $t \in \mathbb{R}$ for arbitrary $\psi \in \mathcal{H}$. Lastly, for $\psi \in \mathcal{H}$:

$$\frac{d}{dt}U_\lambda(t)\psi|_{t=0} = \lim_{t\to 0}\frac{U_\lambda(t)\psi - \psi}{t} = \lim_{t\to 0}\frac{1}{t}\Big(e^{\lambda H R_{i\lambda} t}\psi - \psi\Big) = \lim_{t\to 0}\frac{1}{t}\Big(\sum_{k=0}^{\infty}\frac{\lambda^k t^k}{k!}(HR_{i\lambda})^k\psi - \psi\Big)$$

$$= \lim_{t\to 0}\frac{1}{t}\Big(\sum_{k=1}^{\infty}\frac{\lambda^k t^k}{k!}(HR_{i\lambda})^k\psi\Big) = \lim_{t\to 0}\Big(\lambda H R_{i\lambda}\psi + \sum_{k=2}^{\infty}\frac{\lambda^k t^{k-1}}{k!}(HR_{i\lambda})^k\psi\Big) = \lambda H R_{i\lambda}\psi = -iH_\lambda\psi$$

By the group property and since $R_{i\lambda}H = HR_{i\lambda}$ on $\mathrm{dom}(H)$, we can deduce analogously as in the proof of Theorem (2.2) for all $\psi \in \mathcal{H}$:

$$\frac{d}{dt}U_\lambda(t)\psi = -iH_\lambda U_\lambda(t)\psi = -iU_\lambda(t)H_\lambda\psi \tag{4.5}$$

(3) For fixed $\lambda \in \mathbb{R}$, the group $(U_\lambda(t))_{t\in\mathbb{R}}$ has properties close to the ones we desire for a unitary group. However, the norm is not equal to one for all $t \in \mathbb{R}$ and the differential property is similar to H_λ being the generator instead of H. Thus, we want to take the limit in $\lambda \to \pm\infty$. In order do this, we need to check that $(U_\lambda(t)\psi)_{\lambda\in\mathbb{R}_\pm}$ is a Cauchy sequence for all $\psi \in \mathcal{H}$.
Let $\lambda, \mu \neq 0$, then by the resolvent equality in Theorem (2.7) we have $H_\lambda H_\mu = H_\mu H_\lambda$ and for all $t \in \mathbb{R}$: $H_\mu U_\lambda(t) = U_\lambda(t)H_\mu$. We claim that for $t, s \in \mathbb{R}$:

$$\frac{d}{ds}\big(U_\mu(t-s)U_\lambda(s)\psi\big) = U_\mu(t-s)U_\lambda(s)(-i)(H_\lambda\psi - H_\mu\psi) \tag{4.6}$$

This can be proven with a straight forward calculation:

$$\begin{aligned}
&\frac{d}{ds}\big(U_\mu(t-s)U_\lambda(s)\psi\big) = U_\mu(t)\lim_{h\to 0}\frac{U_\mu(-s+h)U_\lambda(s+h)\psi - U_\mu(-s)U_\lambda(s)\psi}{h}\\
&= U_\mu(t)\lim_{h\to 0}\frac{U_\mu(-s+h)\big(U_\lambda(s+h)-U_\lambda(s)\big)\psi + \big(U_\mu(-s+h)-U_\mu(-s)\big)U_\lambda(s)\psi}{h}\\
&= U_\mu(t)\Big(\lim_{h\to 0}U_\mu(-s+h)\frac{(U_\lambda(s+h)-U_\lambda(s))}{h}\psi + \lim_{h\to\infty}\frac{(U_\mu(-s+h)-U_\mu(-s))}{h}U_\lambda(s)\psi\Big)\\
&= U_\mu(t)\Big(U_\mu(-s)(-iH_\lambda)U_\lambda(s)\psi - (-iH_\mu)U_\mu(-s)U_\lambda(s)\psi\Big) = U_\mu(t-s)U_\lambda(s)(-i)(H_\lambda\psi - H_\mu\psi)
\end{aligned}$$

The first term convergences by a similar calculation as in (2.2) (3).
By the fundamental lemma of calculus:

$$\begin{aligned}
U_\lambda(t)\psi - U_\mu(t)\psi &= \int_0^t \frac{d}{ds}\Big(U_\mu(t-s)U_\lambda(s)\psi\Big)\,ds\\
&= -i\int_0^t U_\mu(t-s)U_\lambda(s)(H_\lambda\psi - H_\mu\psi)\,ds
\end{aligned}$$

By (4.2), if $\psi \in \mathrm{dom}(H)$ then $\|U_\lambda(t)\psi - U_\mu(t)\psi\| \leq |t|\,\|H_\lambda\psi - H_\mu\psi\| \to |t|\,\|H\psi - H\psi\| = 0$ as $\lambda, \mu \to \pm\infty$. Hence, $U_\lambda(t)\psi$ is Cauchy for $\lambda \to \pm\infty, \psi \in \mathrm{dom}(H)$.
We define the forwards time evolution as $U(t)\psi := \lim_{\lambda\to\infty} U_\lambda(t)\psi$ for $t > 0$ and backwards as $U(t)\psi := \lim_{\lambda\to-\infty} U_\lambda(t)\psi$ for $t < 0$ as well as $U(0) = I$, in short

$$U(t)\psi := \lim_{\lambda\to\infty} U_{\mathrm{sign}(t)\lambda}(t)\psi. \tag{4.7}$$

(4) We verify the properties of a unitary group. Since $\|U_{\mathrm{sign}}(\lambda)(t)\| \leq 1$, the limit (4.7) exists for all $\psi \in \mathcal{H}$ and is uniform for t on compact subsets of $\mathbb{R}$, $t \mapsto U(t)\psi$ is continuous on $\mathbb{R}$.
Let $t, s \in \mathbb{R}$ and $\psi \in \mathcal{H}$.

- If $\operatorname{sign}(t) = \operatorname{sign}(s)$, then without loss of generality $t, s > 0$. Using the linearity of $U_\lambda(t)$ for $\lambda > 0$, we get

$$\begin{aligned} 0 &\leq \left\| U_\lambda(t)U_\lambda(s)\psi - U_\lambda(t)\big(\lim_{\mu\to\infty} U_\mu(s)\psi\big) \right\| \leq \|U_\lambda(t)\| \left\| U_\lambda(s)\psi - \lim_{\mu\to\infty} U_\mu(s)\psi \right\| \\ &\leq \left\| U_\lambda(s)\psi - \lim_{\mu\to\infty} U_\mu(s)\psi \right\| \xrightarrow{\lambda\to\infty} 0, \end{aligned}$$

where we used $\|U_\lambda(t)\| \leq 1$ for all $\lambda, t > 0$ and the continuity of the norm. We obtain:

$$\begin{aligned} U(t+s)\psi &= \lim_{\lambda\to\infty} U_\lambda(t+s)\psi = \lim_{\lambda\to\infty} U_\lambda(t)U_\lambda(s)\psi = \lim_{\lambda\to\infty} U_\lambda(t)\big(\lim_{\mu\to\infty} U_\mu(s)\psi\big) \\ &= U(t)U(s)\psi \end{aligned}$$

- If $t + s = 0$, then without loss of generality $t = -s > 0$ and analogously

$$\begin{aligned} 0 &\leq \left\| U_\lambda(t)U_{-\lambda}(-t)\psi - U_\lambda(t)\big(\lim_{\mu\to\infty} U_{-\mu}(-t)\psi\big) \right\| \leq \|U_\lambda(t)\| \left\| U_{-\lambda}(-t)\psi - \lim_{\mu\to\infty} U_{-\mu}(-t)\psi \right\| \\ &\leq \left\| U_{-\lambda}(-t)\psi - \lim_{\mu\to\infty} U_{-\mu}(-t)\psi \right\| \xrightarrow{\lambda\to\infty} 0. \end{aligned}$$

This implies

$$U(t)U(s)\psi = \lim_{\lambda\to\infty} U_\lambda(t) \lim_{\mu\to\infty} U_{-\mu}(-t)\psi = \lim_{\lambda\to\infty} U_\lambda(t)U_{-\lambda}(-t)\psi. \tag{4.8}$$

A special case of Equation (4.6) for $t = 0$ gives

$$\frac{d}{ds}(U_\lambda(s)U_{-\lambda}(-s)\psi) = U_\lambda(s)U_{-\lambda}(-s)(-i)(H_\lambda\psi - H_{-\lambda}\psi)$$

for all $s \in \mathbb{R}$. Then

$$\left\| \frac{d}{dt}(U_\lambda(t)U_{-\lambda}(-t)\psi) \right\| \leq \|U_\lambda(t)\| \, \|U_{-\lambda}(-t)\| \, \|H_\lambda\psi - H_{-\lambda}\psi\| \xrightarrow{\lambda\to\infty} 0,$$

since $\|U_\lambda(t)\|, \|U_{-\lambda}(-t)\| \leq 1$ and $H_\lambda\psi \to H\psi$ as $\lambda \to \pm\infty$. As the convergence in 4.8 is uniform on compact subsets of $\mathbb{R}$, the derivative converges as well. We obtain

$$\frac{d}{dt}\big(\lim_{\lambda\to\infty} U_\lambda(t)U_{-\lambda}(-t)\psi\big) = \lim_{\lambda\to\infty} \big(\frac{d}{dt} U_\lambda(t)U_{-\lambda}(-t)\psi\big) = 0,$$

so $\lim_{\lambda\to\infty} U_\lambda(t)U_{-\lambda}(-t)\psi$ is constant in t. With $U_\lambda(0) = I$ for all $\lambda \in \mathbb{R}$,

$$\lim_{\lambda\to\infty} U_\lambda(t)U_{-\lambda}(-t)\psi = \lim_{\lambda\to\infty} U_\lambda(0)U_{-\lambda}(0)\psi = \psi.$$

Therefore,

$$U(t)U(s)\psi = \lim_{\lambda\to\infty} U_\lambda(t) \lim_{\mu\to\infty} U_{-\mu}(-t)\psi = \lim_{\lambda\to\infty} U_\lambda(t)U_{-\lambda}(-t)\psi = \psi = U(t+s)\psi$$

- If $\operatorname{sign}(t) \neq \operatorname{sign}(s)$, then without loss of generality $t+s, -t, s > 0$. From the two cases above:

$$U(-t)U(t+s)\psi = U(t-t+s)\psi = U(s)\psi,$$

so $U(t+s)\psi = U(t)U(-t)U(t+s)\psi = U(t)U(s)\psi$.

Hence, $U(t+s) = U(t)U(s)$. The operator norm is continuous, so we obtain $\|U(t)\| \leq 1$. Then

$$1 = \|U(0)\| = \|U(t)U(-t)\| \leq \|U(t)\| \, \|U(-t)\| \leq \|U(t)\| \leq 1,$$

so $\|U(t)\| = 1$ for all $t \in \mathbb{R}$. Therefore $(U(t))_{t\in\mathbb{R}}$ is a strongly continuous group.
It remains to prove that its generator is H. Denote by B the generator of the group, which exists by the first part of the theorem, then

$$U_\lambda(t)\psi - \psi = -i \int_0^t U_\lambda(s) H_\lambda \psi ds.$$

For $\psi \in \operatorname{dom}(H)$:

$$\|U_\lambda(s)H_\lambda\psi - U(s)H\psi\| \leq \|U_\lambda(s)\| \, \|H_\lambda\psi - H\psi\| + \|(U_\lambda(s) - U(s))H\psi\| \to 0$$

as $\lambda \to \infty$. Taking the limit, we get

$$U(t)\psi - \psi = -i \int_0^t U(s)H\psi \, ds$$

where we can interchange the limit and integral using the Dominated Convergence Theorem since $s \to U(s)H\psi$ is continuous and therefore bounded on the compact set $[0,t]$. Therefore, the limit

$$B\psi = i \lim_{t\to 0} \frac{U(t)\psi - \psi}{t} = H\psi.$$

exists, so $\operatorname{dom}(H) \subseteq \operatorname{dom}(B)$.
If $\lambda > 0$, then $i\lambda \in \rho(H)$ according to (4.1) and B is a generator of a unitary group, thus by the first part of the Theorem, $i\lambda \in \rho(B)$. Then $\operatorname{ran}(i\lambda - H) = \mathcal{H}$, so for any $\varphi \in \operatorname{dom}(B)$ there exists $\psi \in \operatorname{dom}(H)$ such that $(i\lambda - B)\varphi = (i\lambda - H)\psi$. As B is an extension of H and $(i\lambda - B)$ is bijective, we get $(i\lambda - B)\varphi = (i\lambda - B)\psi$ and $\varphi = \psi \in \operatorname{dom}(H)$. Therefore, $\operatorname{dom}(H) = \operatorname{dom}(B)$ and $H = B$ is indeed the generator of the group $(U(t))_{t\in\mathbb{R}}$. □

In the setting of the Schrödinger equation this means: If there is a solution with constant norm for all initial values $\psi \in \operatorname{dom}(H)$, then the generator H is self-adjoint on $\operatorname{dom}(H)$. Conversely, if a self-adjoint Hamiltonian operator H is given, then there is a unique solution for all initial states in its domain. Typically, the Hamiltonian coincides with the total energy of a quantum system and can be derived from the physical setting.

5 Stone's Theorem

With the help of the operator theory covered in Chapter 3, we use another method to prove a special case of the Hille-Yosida Theorem for Hilbert spaces. This chapter is inspired by Section 4 in [6]. We focus on the initial value problem from Section 2:

$$i\frac{d\psi(t)}{dt} = H\psi(t) \text{ for all } t \in \mathbb{R} \quad \text{with the initial condition } \psi(0) = \psi_0 \in \mathrm{dom}(H) \tag{5.1}$$

where the Hamilton operator $H : \mathrm{dom}(H) \subseteq \mathcal{H} \to \mathcal{H}$ is densely defined. If solutions exist, they can be described with the help of a unitary group with generator H. Remember that a solution of the differential equation (5.1) is a differentiable function $\psi : I \to \mathcal{H}$ on a nontrivial open interval $I \in \mathbb{R}$ with $0 \in I$ that satisfies

(1) $\forall t \in I : \psi(t) \in \mathrm{dom}(H)$,

(2) $i\frac{d}{dt}\psi(t) := \lim_{h\to 0} i\frac{\psi(t+h) - \psi(t)}{h} = H\psi(t)$,

(3) $\lim t \to 0\psi(t) = \psi_0$.

First, we study some basic connections between the existence of a solution and the operator H before we move on to the special case of Hille-Yosida. Remember that for a wave function $\psi(t)$, the squared absolute value $|\psi(t)|^2$ is interpreted as a probability measure, so it makes sense to ask for constant norm.

Theorem 5.1.

(1) If equation (5.1) has a solution $\psi(t)$ with constant norm for all initial values $\psi(0) = \psi \in \mathrm{dom}(H)$, then H is symmetric.

(2) If H is symmetric, then equation (5.1) has a at most one solution (locally). This solution has constant norm.

Proof.

(1) Let $\psi(t)$ be a solution with constant norm for an arbitrary $\psi(0) = \psi \in \mathrm{dom}(H)$. Then

$$\begin{aligned} 0 =& \frac{d}{dt}\langle \psi(t), \psi(t)\rangle = \left\langle \frac{d}{dt}\psi(t), \psi(t)\right\rangle + \left\langle \psi(t), \frac{d}{dt}\psi(t)\right\rangle \\ &= \langle -iH\psi(t), \psi(t)\rangle + \langle \psi(t), -iH\psi(t)\rangle = i\langle H\psi(t), \psi(t)\rangle - i\langle \psi(t), H\psi(t)\rangle \end{aligned}$$

This implies $\langle \psi(t), H\psi(t)\rangle = \langle H\psi(t), \psi(t)\rangle$ for all $t \in \mathbb{R}$, in particular for $t = 0$. Hence, for all $\psi \in \mathrm{dom}(H) : \langle \psi, H\psi\rangle = \langle H\psi, \psi\rangle$. With the polarization identity we get $\langle \psi, H\varphi\rangle = \langle H\psi, \varphi\rangle$ for all $\psi, \varphi \in \mathrm{dom}(H)$, so H is symmetric.

(2) Let $\psi(t), \tilde{\psi}(t)$ be two solutions for the initial value $\psi \in \mathrm{dom}(H)$, then

$$i\frac{d}{dt}(\psi(t) - \tilde{\psi}(t)) = H(\psi(t) - \tilde{\psi}(t)) \quad \text{and} \quad (\psi(0) - \tilde{\psi}(0)) = 0$$

By the same calculation as above we get $\frac{d}{dt}\left\langle \psi(t)-\tilde{\psi}(t), \psi(t)-\tilde{\psi}(t)\right\rangle = 0$. Hence, the inner product is constant in t. Setting $t=0$, this implies

$$\left\|\psi(t)-\tilde{\psi}(t)\right\| = \left\|\psi(0)-\tilde{\psi}(0)\right\| = 0 \implies \psi(t) = \tilde{\psi}(t).$$

Thus, there is at most one solution for each $t \in \mathbb{R}$. Furthermore, we see that the norm of every solution is constant if H is symmetric. □

Combining the two statements, we know that if there is a solution with constant norm, that is the norm of the initial value, for all initial values $\psi \in \mathcal{H}$, then every solution is unique. Next, we introduce a weaker version of the self-adjointness property which uses the closure of an operator.

Definition 5.1. A densely defined, symmetric and therefore closable operator A is called essentially self-adjoint if its closure $\overline{A}$ is self-adjoint.

There are criteria for essential self-adjointness of an operator similar to the ones we found for self-adjointness:

Theorem 5.2. Let $A : \mathrm{dom}(A) \to \mathcal{H}$ be a densely defined, symmetric operator. Then the following assertions are equivalent:

(1) A is essentially self-adjoint.

(2) $\overline{\mathrm{ran}(A - z_\pm)} = \mathcal{H}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$

(3) $\ker(A^* - z_\pm) = \{0\}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$

Proof.

- (1) $\implies$ (3): $\overline{A}$ is self-adjoint by assumption and $\left(\overline{A}^* = A^*\right)$ by Theorem (3.5). So $\ker(A^* - z_\pm) = \ker\left(\overline{A}^* - z_\pm\right)$ and with Theorem (3.8) $\ker(A^* - z_\pm) = \{0\}$.
- (3) $\implies$ (2): With Theorem (3.6) we get: $\mathrm{ran}(A - z_\pm)^\perp = \ker(A^* - z_\pm) = \{0\}$.
- (2) $\implies$ (1): Since A is symmetric, A is closable with closure $\overline{A}$. We prove $\overline{\mathrm{ran}(A - z_\pm)} \subseteq \mathrm{ran}(\overline{A} - z_\pm)$, then $\mathrm{ran}(\overline{A} - z_\pm) = \mathcal{H}$, so by Theorem (3.8) $\overline{A}$ is self-adjoint.

  Since $\mathrm{ran}(A - z_\pm) \subseteq \mathrm{ran}\left(\overline{A} - z_\pm\right)$, it remains to prove that $\mathrm{ran}\left(\overline{A} - z_\pm\right)$ is closed. This is done analogously to the proof of Theorem (3.8) (2) $\implies$ (3). □

We apply this to the generator of the unitary group which is induced by the existing solutions as in Definition (2.2).

Theorem 5.3. If H is symmetric and equation (5.1) has a solution in $I = \mathbb{R}$ for all initial conditions $\psi \in \mathrm{dom}(H)$, then H is essentially self-adjoint.

Proof. We prove $\ker(H^* \pm i) = \{0\}$, then H is essentially self-adjoint by Theorem (5.2). Let $\psi(t)$ be a solution of (5.1) for the initial condition $\psi \in \mathrm{dom}(H)$ and $\varphi \in \ker(H^* + i)$, then $H^*\varphi = -i\varphi$. Then

$$\frac{d}{dt}\langle \varphi, \psi(t)\rangle = \langle \varphi, -iH\psi(t)\rangle = \langle iH^*\varphi, \psi(t)\rangle = \langle \varphi, \psi(t)\rangle$$

Solving this differential equation, we find $\langle \varphi, \psi(t)\rangle = e^t \left(\langle \varphi, \psi(t)\rangle\right)|_{t=0} = e^t \langle \varphi, \psi(0)\rangle = e^t \langle \varphi, \psi\rangle$. By Cauchy-Schwary and Theorem (5.1) we have $|\langle \varphi, \psi(t)\rangle| \leq \|\varphi\| \|\psi(t)\| \leq \|\varphi\| \|\psi\|$. Therefore $\left|e^t \langle \varphi, \psi\rangle\right| \leq \|\varphi\| \|\psi\|$ holds for all $t \in \mathbb{R} \implies \langle \varphi, \psi\rangle = 0$ for all $\psi \in \mathrm{dom}(H)$. Since $\mathrm{dom}(H)$ is dense in $\mathcal{H}$ we get $\varphi = 0$. □

We are interested in solutions $\psi(t) = U(t)\psi$ such that $U(t)$ is a strongly continuous unitary group with generator H. Again, we want to prove self-adjointness of H.

Theorem 5.4. Let $H : \mathrm{dom}(H) \to \mathcal{H}$ be the generator of a strongly continuous unitary group $(U(t))_{t\in\mathbb{R})}$ defined by (2.8). Then:

(1) $U(t)\mathrm{dom}(H) \subseteq \mathrm{dom}(H)$ and for all $\psi \in \mathrm{dom}(H) : i\frac{d}{dt}U(t)\psi = HU(t)\psi = U(t)H\psi$

(2) H is self-adjoint.

(3) $U(t)$ is uniquely determined by H.

Proof. We have already seen parts of this Theorem, however for completeness we will give all proofs here again.

(1) For $\psi \in \mathrm{dom}(H)$ we have:

$$i \lim_{h\to 0} \frac{U(t+h)\psi - U(t)\psi}{h} = U(t) i \lim_{h\to 0} \frac{U(h) - I}{h}\psi = U(t)H\psi$$

Thus, $U(t)\psi \in \mathrm{dom}(H)$ and $HU(t)\psi = i\frac{d}{dt}U(t)\psi = HU(t)\psi$.

(2) We proceed in the following steps:

  (1) H is densely defined.
  (2) H is symmetric.
  (3) H is essentially self-adjoint.
  (4) H is self-adjoint.

(1) This is Theorem (2.5) (1).

(2) We prove that $\langle \psi, H\varphi\rangle = \langle H\psi, \varphi\rangle$ for all $\psi, \varphi \in \mathrm{dom}(H)$. Using the continuity of the inner product we get

$$\langle \psi, H\varphi\rangle = \lim_{h\to 0} \left\langle \psi, i\frac{U(h) - I}{h}\varphi \right\rangle = \lim_{h\to 0} \left\langle -i\frac{U(-h) - I}{h}\psi, \varphi \right\rangle = \lim_{h\to 0} \left\langle i\frac{U(-h) - I}{-h}\psi, \varphi \right\rangle$$
$$= \langle H\psi, \varphi\rangle$$

(3) H is symmetric and by (1), equation (5.1) has a solution for all times. Thus, by Theorem (5.3) H is essentially self-adjoint.

(4) By Theorem (2.5) (2) H is closed, so $H = \overline{H}$ is self-adjoint.

(3) Let $\psi \in \operatorname{dom}(H)$. Then

$$\begin{aligned}\frac{d}{dt}\left\|[U(t)-\tilde{U}(t)]\psi\right\|^2 &= 2\frac{d}{dt}\left[\|\psi\|^2 - \operatorname{Re}\left\langle U(t)\psi, \tilde{U}(t)\psi\right\rangle\right]\\ &= -2\operatorname{Re}\left[\left\langle -iHU(t)\psi, \tilde{U}(t)\psi\right\rangle + \left\langle U(t)\psi, -iH\tilde{U}(t)\psi\right\rangle\right]\\ &= -2\operatorname{Re}\left[i\left\langle HU(t)\psi, \tilde{U}(t)\psi\right\rangle - i\left\langle U(t)\psi, H\tilde{U}(t)\psi\right\rangle\right] = 0\end{aligned}$$

The last term equals zero since H is symmetric by (2). This implies the uniqueness of $U(t)$ since

$$\left\|[U(t)-\tilde{U}(t)]\psi\right\| = \left\|[U(0)-\tilde{U}(0)]\psi\right\| = \|[I-I]\psi\| = 0$$

by the definition of a unitary group. This implies $U(t) = \tilde{U}(t)$ for all times $t \in \mathbb{R}$. □

This is part of the result from Theorem (4.1), since the resolvent properties (2.15) are equivalent to H being self-adjoint, as we have seen at the end of Chapter 3.
Conversely, with a given self-adjoint H we are able construct a unitary group with H as its generator. First, assume that H is bounded.

Theorem 5.5 (Bounded case)**.** Let $H : \mathcal{H} \to \mathcal{H}$ be bounded and self-adjoint. Then equation (5.1) has the unique solution $\psi(t) = e^{-iHt}\psi$ for all $\psi \in \operatorname{dom}(H) = \mathcal{H}$, with

$$e^{-iHt} := \sum_{k=0}^{\infty} \frac{(-iHt)^k}{k!}.$$

where the limit is taken with respect to the operator norm. This solution is well-defined and global in time. The map $U : \mathbb{R} \to \operatorname{BL}(\mathcal{H}), U(t) = e^{-iHt}$ satisfies

(1) $U(t)$ is unitary, $U(t)U(s) = U(t+s)$ for all $t, s \in \mathbb{R}$ and $U(0) = I$,

(2) $\lim_{t\to 0} U(t)\psi = \psi$ for all $\psi \in \mathcal{H}$.

Proof. We used a similar approach before in the proof of the Hille-Yosida Theorem, where we have seen that the exponential e^{-iHt} with H bounded is well-defined. The solution is well-defined since $\|H\varphi\| \le \|H\|\,\|\varphi\|$ for all $\varphi \in \mathcal{H}$ by boundedness, so

$$\|\psi(t)\| = \left\|\sum_{k=0}^{\infty}\frac{(-iHt)^k}{k!}\psi\right\| \le \sum_{k=0}^{\infty}\frac{|t|^k}{k!}\left\|H^k\psi\right\| \le \sum_{k=0}^{\infty}\frac{|t|^k}{k!}\|H\|^k\|\psi\| = e^{\|H\||t|}\|\psi\|$$

We check the group properties of $U(t)$:

(1) Let $t, s \in \mathbb{R}$. Since the sum converges in operator norm, we can change the order of summation. With the Cauchy product and the binomial formula:

$$\begin{aligned}U(t)U(s) &= \Big(\sum_{k=0}^{\infty}\frac{(-iHt)^k}{k!}\Big)\Big(\sum_{l=0}^{\infty}\frac{(-iHs)^l}{l!}\Big) = \sum_{m=0}^{\infty}\sum_{k+l=m}\frac{(-iHt)^k}{k!}\frac{(-iHs)^l}{l!}\\ &= \sum_{m=0}^{\infty}(-iH)^m\sum_{k=0}^{m}\frac{1}{k!(m-k)!}t^k s^{m-k} = \sum_{m=0}^{\infty}(-iH)^m\sum_{k=0}^{m}\frac{1}{m!}\binom{m}{k}t^k s^{m-k}\\ &= \sum_{m=0}^{\infty}\frac{(-iH(t+s))^m}{m!} = U(t+s)\end{aligned}$$

Furthermore

$$U^*(t) = \Big(\sum_{k=0}^{\infty} \frac{(-iHt)^k}{k!}\Big)^* = \sum_{k=0}^{\infty} \frac{(iHt)^k}{k!} = U(-t)$$

So $U^*(t)U(t) = U(-t)U(t) = U(0) = I$ by definition, so $U(t)$ is unitary.

(2) We have

$$U(t)\psi - \psi = \sum_{k=1}^{\infty} \frac{(-iHt)^k}{k!}\psi = -iHt\sum_{k=1}^{\infty} \frac{(-iHt)^{k-1}}{k!}\psi$$

$$\implies \|U(t)\psi - \psi\| \le |t|\,\|H\| \left\|\sum_{k=1}^{\infty} \frac{(-iHt)^{k-1}}{k!}\psi\right\| \xrightarrow{t\to 0} 0 \implies U(t)\psi - \psi \xrightarrow{t\to 0} 0$$

Now we prove $\psi(t) = U(t)\psi = e^{-iHt}\psi$ is indeed a solution of (5.1) for all $t \in \mathbb{R}$. The uniqueness of the solution follows from Theorem (5.1) since H is self-adjoint, so in particular symmetric. Trivially $\psi(0) = e^{-iH\cdot 0}\psi = \psi$. We calculate

$$i\frac{d}{dt}\psi(t) = i\lim_{h\to 0}\frac{U(t+h)\psi - U(t)\psi}{h} = i\lim_{h\to 0}\frac{U(h)U(t)\psi - U(t)\psi}{h} = i\lim_{h\to 0}\frac{U(h)-I}{h}U(t)\psi$$

$$= \lim_{h\to 0}\Big(\frac{U(h)-I}{h}\Big)\psi(t)$$

and

$$\lim_{h\to 0}\Big(\frac{U(h)-I}{h}\Big)\psi(t) = \frac{i}{h}\sum_{k=1}^{\infty}\frac{(-iHh)^k}{k!}\psi(t) = \frac{i(-iHh)}{h}\sum_{k=1}^{\infty}\frac{(-iHh)^{k-1}}{k!}\psi(t) \xrightarrow{h\to 0} H\psi(t),$$

so indeed $i\frac{d}{dt}\psi(t) = H\psi(t)$ and $\psi(0) = \psi$. □

Theorem 5.6. $(U(t))_{t\in\mathbb{R}}$ from Theorem (5.5) is a strongly continuous unitary group by definition (2.2).

Proof. The two conditions in (5.5) imply that $t \mapsto U(t)\varphi$ is continuous for $t \in \mathbb{R}$ and all $\varphi \in \mathcal{H}$:

$$\lim_{h\to 0} U(t+h)\varphi - U(t)\varphi = \lim_{h\to 0}(U(h) - I)U(t)\varphi = 0$$

Therefore, with (5.5) (1) all conditions of a strongly continuous unitary group are satisfied. □

Hence, we found a strongly continuous group with a bounded operator H as its generator. It remains to extend this construction to the unbounded case. Remember that in order to study unbounded operators, it is reasonable to study the bounded resolvent operator first. For this, we prove an approximation of its norm.

Lemma 5.7. Let $H : \mathrm{dom}(H) \to \mathcal{H}$ be self-adjoint. For $\lambda, \mu \in \mathbb{R}, \mu \neq 0$:

$$\|R_{\lambda+i\mu}\| \le \frac{1}{|\mu|}$$

Proof. By Theorem (3.9) for $\varphi \in \operatorname{dom}(H)$:

$$\|(H-\lambda-i\mu)\varphi\|^2 = \|H\varphi\|^2 + \mu^2\|\varphi\|^2 \geq \mu^2\|\varphi\|^2 \quad \Longrightarrow \|(H-\lambda-i\mu)\varphi\| \geq |\mu|\,\|\varphi\|$$

For $\psi \in \mathcal{H}$ we have $\varphi = (H-\lambda-i\mu)^{-1}\psi \in \operatorname{dom}(H)$, so

$$\left\|(H-\lambda-i\mu)^{-1}\psi\right\| = \|\varphi\| \leq \frac{1}{|\mu|}\|(H-\lambda-i\mu)\varphi\| = \frac{1}{|\mu|}\|\psi\|.$$

Hence, $\left\|(H-\lambda-i\mu)^{-1}\right\| = \sup_{\psi\in\mathcal{H}} \frac{\left\|(H-\lambda-i\mu)^{-1}\psi\right\|}{\|\psi\|} \leq \frac{1}{|\mu|}$. □

In order to generalize the bounded case, we will define a sequence of bounded operators H_λ on $\mathcal{H}$ that approximate the unbounded operator H on $\operatorname{dom}(H)$. For these operators, we can explicitly write the generated unitary groups. Taking the limit $\lambda \to \infty$ provides the unitary group with generator H we desire.

Theorem 5.8 (General case)**.** Let $H : \operatorname{dom}(H) \to \mathcal{H}$ be self-adjoint. Then equation (5.1) has a unique solution that is global in time. There exists a strongly continuous unitary group $U(t)$ such that for all $t \in \mathbb{R}$ and $\psi \in \operatorname{dom}(H) : \psi(t) = U(t)\psi$.

Proof. If the solution exists, its uniqueness is already proven. Let $B_\lambda : \mathcal{H} \to \operatorname{dom}(H), B_\lambda := i\lambda(H+i\lambda)^{-1}$ and $H_\lambda : \mathcal{H} \to \operatorname{dom}(H), H_\lambda := B_\lambda H B_{-\lambda}$. If H were a real number, we would have $\lim_{\lambda\to\pm\infty} B_\lambda = 1$. Informally, we hope for $\lim_{\lambda\to\pm\infty} B_\lambda = I$ and $\lim_{\lambda\to\pm\infty} H_\lambda = H$ in a certain sense. We will prove the theorem in the following steps:

(1) H_λ is bounded and self-adjoint for all $\lambda \geq 1$.

(2) $H_\lambda\psi \to H\psi$ as $\lambda \to \infty$ for all $\psi \in \operatorname{dom}(H)$

(3) $\lim\limits_{\lambda\to\infty} e^{-iH_\lambda t}\psi$ exists for all $\psi \in \operatorname{dom}(H)$ and for fixed $\psi \in \operatorname{dom}(H)$ the limit is uniform on compact sets $[-N, N]$ for all $N > 0$.

(4) $\lim\limits_{\lambda\to\infty} e^{-iH_\lambda t}\psi$ exists for all $\psi \in \mathcal{H}$ and $U : \mathbb{R} \to \mathrm{BL}(\mathcal{H})$ with $U(t)\psi = \lim\limits_{\lambda\to\infty} e^{-iH_\lambda t}\psi$ is a strongly continuous unitary group.

(5) $\psi(t) := U(t)\psi$ is a solution of (5.1).

(1) $B_{\pm\lambda}$ is bounded since $\pm i\lambda \in \rho(H)$ for all $\lambda \geq 1 : \|B_{\pm\lambda}\| = \lambda\|R_{\pm i\lambda}\|$. Note that $B_\lambda^* = (i\lambda(H+i\lambda)^{-1})^* = -i\lambda(H-i\lambda)^{-1} = B_{-\lambda}$. By Theorem (3.9) we have $\|(H-i\lambda)\varphi\|^2 = \|H\varphi\|^2 + \lambda^2\|\varphi\|^2 \geq \|H\varphi\|^2$, so $\|H\varphi\| \leq \|(H-i\lambda)\varphi\|$ for all $\varphi \in \operatorname{dom}(H)$.
For $\psi \in \mathcal{H}$ we have $\varphi = (H-i\lambda)^{-1}\psi \in \operatorname{dom}(H)$ and therefore $\left\|H(H-i\lambda)^{-1}\psi\right\| = \|H\varphi\| \leq \|(H-i\lambda)\varphi\| = \left\|(H-i\lambda)(H-i\lambda)^{-1}\psi\right\| = \|\psi\|$. Thus $\left\|H(H-i\lambda)^{-1}\right\| \leq 1$. We get

$$\|H_\lambda\| = \|B_\lambda H B_{-\lambda}\| \leq \|B_\lambda\|\left\|H\, i\lambda(H-i\lambda)^{-1}\right\| \leq \lambda\|B_\lambda\|\left\|H\,(H-i\lambda)^{-1}\right\| \leq \lambda\|B_\lambda\|,$$

so H_λ is bounded. Let $\varphi, \psi \in \mathcal{H}$, then

$$\begin{aligned}\langle\varphi, H_\lambda\psi\rangle &= \langle\varphi, B_\lambda H B_{-\lambda}\psi\rangle = \langle B_{-\lambda}\varphi, H B_{-\lambda}\psi\rangle = \langle H B_{-\lambda}\varphi, B_{-\lambda}\psi\rangle = \langle B_\lambda H B_{-\lambda}\varphi, \psi\rangle \\ &= \langle H_\lambda\varphi, \psi\rangle\end{aligned}$$

We use symmetry of H with $B_{-\lambda}\varphi, B_{-\lambda}\psi \in \operatorname{dom}(H)$. Hence, H_λ is self-adjoint.
(2) We prove $\lim_{\lambda\to\infty} B_{\pm\lambda}\varphi = \varphi$ for all $\varphi \in \operatorname{dom}(H)$.With Lemma (4.2), we have

$$B_\lambda\varphi - \varphi = i\lambda(H+i\lambda)^{-1}\varphi - (H+i\lambda)(H+i\lambda)^{-1}\varphi = -H(H+i\lambda)^{-1}\varphi = -(H+i\lambda)^{-1}H\varphi$$

Therefore,

$$\|B_\lambda\varphi - \varphi\| \leq \left\|(H+i\lambda)^{-1}\right\| \|H\varphi\| \leq \frac{1}{|\lambda|}\|H\varphi\| \xrightarrow{\lambda\to\infty} 0$$

with Lemma (5.7). Similarly for $B_{-\lambda}$. Let $\psi \in \mathcal{H}$, $\varphi \in \operatorname{dom}(H)$, $\varepsilon > 0$ with $\|\psi - \varphi\| < \frac{\varepsilon}{3}$. Then

$$\|B_\lambda\psi - \psi\| = \|B_\lambda\psi - B_\lambda\varphi + B_\lambda\varphi - \varphi + \varphi - \psi\| \leq (\|B_\lambda\| + 1)\|\psi - \varphi\| + \|B_\lambda\varphi - \varphi\|$$

$$\leq \frac{2\varepsilon}{3} + \|B_\lambda\varphi - \varphi\|$$

since $\|B_\lambda\| = |\lambda|\left\|(H+i\lambda)^{-1}\right\| \leq 1$, with Lemma (5.7). Hence, $B_{\pm\lambda}\psi - \psi \to 0$ as $\lambda \to \infty$ for all $\psi \in \mathcal{H}$. By Lemma (4.2), for $\psi \in \operatorname{dom}(H) : H_\lambda\psi = B_\lambda H B_{-\lambda}\psi = B_\lambda B_{-\lambda}H\psi$. Therefore, $H_\lambda\psi - H\psi = B_\lambda B_{-\lambda}H\psi - B_\lambda H\psi + B_\lambda H\psi - H\psi = B_\lambda(B_{-\lambda}H\psi - H\psi) + B_\lambda H\psi - H\psi$. We have $B_{\pm\lambda}H\psi - H\psi \to 0$ as $\lambda \to \infty$. B_λ is uniformly bounded for $\lambda \to \infty$, so $H_\lambda\psi - H\psi \to 0$.
(3) Let $\lambda, \mu \geq 1$. By Theorem (5.5):

$$\frac{d}{dt}e^{-iH_\lambda t}\psi = e^{-iH_\lambda t}(-iH_\lambda)\psi = -iH_\lambda e^{-iH_\lambda t}\psi$$

By Theorem (5.6) $U_\mu(t) := e^{-iH_\mu t}$ is unitary, so $U_\mu(t)U_\mu(-t) = e^{-iH_\mu t}e^{iH_\mu t} = I$. For $\psi \in \operatorname{dom}(H)$:

$$\left\|e^{-iH_\lambda t}\psi - e^{-iH_\mu t}\psi\right\| = \left\|e^{-iH_\mu t}\big(e^{iH_\mu t}e^{-iH_\lambda t}\psi - \psi\big)\right\| = \left\|e^{iH_\mu t}e^{-iH_\lambda t}\psi - \psi\right\|$$

The fundamental lemma of calculus gives:

$$e^{iH_\mu t}e^{-iH_\lambda t}\psi - \psi = \int_0^t \frac{d}{ds}\big(e^{iH_\mu s}e^{-iH_\lambda s}\psi\big)\,ds = \int_0^t e^{iH_\mu s}(iH_\mu - iH_\lambda)e^{-iH_\lambda s}\psi\,ds$$

$$= \int_0^t e^{iH_\mu s}e^{-iH_\lambda s}(iH_\mu - iH_\lambda)\psi\,ds$$

Therefore, $\left\|e^{iH_\mu s}e^{-iH_\lambda s}\psi - \psi\right\| \leq |t|\,\|(H_\lambda - H_\mu)\psi\| \leq N\,\|(H_\lambda - H_\mu)\psi\|$ for $t \in [-N, N]$ for all $N > 0$. $\implies \left\|e^{-iH_\lambda t}\psi - e^{-iH_\mu t}\psi\right\| \leq N\,\|(H_\lambda - H_\mu)\psi\| \xrightarrow{\lambda,\mu\to\infty} 0$ since $H_\lambda\psi \xrightarrow{\lambda\to\infty} H\psi$. Hence $e^{-iH_\lambda t}\psi$ is uniformly Cauchy in $t \in [-N, N]$ and thus uniformly convergent.
(4) Let $t \in \mathbb{R}$ and $\lambda, \mu \geq 1$. For $\psi \in \mathcal{H}$:

$$\left\|e^{-iH_\lambda t}\psi - e^{-iH_\mu t}\psi\right\| = \left\|e^{iH_\mu t}e^{-iH_\lambda t}\psi - \psi\right\|$$

We write $U_{\mu,\lambda}(t) := e^{iH_\mu t}e^{-iH_\lambda t}$ with $\|U_{\mu,\lambda}(t)\| \leq 1$.
Let $\varepsilon > 0$. H is densely defined, so there is $\varphi \in \operatorname{dom}(H)$ with $\|\psi - \varphi\| < \frac{\varepsilon}{3}$. Then

$$\|U_{\mu,\lambda}(t)\psi - \psi\| = \|U_{\mu,\lambda}(t)(\psi - \varphi) + U_{\mu,\lambda}(t)\varphi - \varphi + \varphi - \psi\|$$

$$= \|(U_{\mu,\lambda}(t) - I)(\psi - \varphi)\| + \|U_{\mu,\lambda}(t)\varphi - \varphi\|$$

$$\leq (\|U_{\mu,\lambda}(t)\| + 1)\|\psi - \varphi\| + \|U(t)\varphi - \varphi\| \leq \frac{2\varepsilon}{3} + \|U_{\mu,\lambda}(t)\varphi - \varphi\|$$

By (3) we can choose $M \geq 1$ such that for all $\lambda, \mu \geq M$: $\|U_{\mu,\lambda}(t)\varphi - \varphi\| < \frac{\varepsilon}{3}$. Then $\left\|e^{-iH_\lambda t}\psi - e^{-iH_\mu t}\psi\right\| < \varepsilon$, so $e^{-iH_\lambda t}\psi$ is Cauchy.

First we prove the group property $U(t+s) = U(t)U(s)$ on $\mathcal{H}$. Let $\varphi \in \operatorname{dom}(H)$ and write $U_\lambda(t) = e^{-iH_\lambda t}$. By Theorem (5.5) $U_\lambda(t+s)\psi = U_\lambda(t)U_\lambda(s)\psi$. We have $U_\lambda(t+s)\psi \to U(t+s)\psi$ and $U_\lambda(t)U_\lambda(s)\psi \to U(t)U(s)\psi$ as $\lambda \to \infty$ since

$$U_\lambda(t)U_\lambda(s)\psi - U(t)U(s)\psi = U_\lambda(t)(U_\lambda(s)\psi - U(s)\psi) + (U_\lambda(t) - U(t))U(s)\psi \to 0$$

by (3) and with $\|U_\lambda(t)\| \leq 1$. By an analogous approximation argument as before the same result follows for $\psi \in \mathcal{H}$.

Now we prove that $U(t)$ is unitary. Let $\psi \in \mathcal{H}$, then by continuity of the norm for all $t \in \mathbb{R}$:

$$\|U(t)\psi\| = \lim_{\lambda\to\infty} \|U_\lambda(t)\psi\| = \lim_{\lambda\to\infty} \|\psi\| = \|\psi\|$$

For the strong continuity it suffices to prove continuity for all $\psi \in \operatorname{dom}(H)$ since $\operatorname{dom}(H)$ is dense in $\mathcal{H}$.

Let $f_\lambda(t) := U_\lambda(t)\psi$ for all $t \in \mathbb{R}$. Then $f_\lambda(t)$ is continuous by Theorem (5.6). By (3) we have $f_\lambda(t) \to U(t)\psi$ uniformly in $[-N, N]$ for all $N > 0$. Since f_λ is continuous for all λ the limit function $U(t)\psi$ is continuous.

(5) Let $\psi(t) := U(t)\psi$. We want to prove that $\psi(t)$ is a solution of the differential equation (5.1) for all $\psi \in \operatorname{dom}(H)$. We have:

$$i\frac{d}{dt}\psi(t) = i\lim_{h\to 0}\frac{U(t+h)\psi - U(t)\psi}{h} = iU(t)\lim_{h\to 0}\frac{U(h) - I}{h}\psi$$

For fixed $h \neq 0$,

$$\frac{U(h) - I}{h}\psi = \lim_{\lambda\to\infty}\frac{U_\lambda(t) - U_\lambda(0)}{h}\psi = \lim_{\lambda\to\infty}\frac{1}{h}\int_0^h \frac{d}{ds}\big(U_\lambda(s)\psi\big)\,ds = \lim_{\lambda\to\infty}\frac{1}{h}\int_0^h U_\lambda(s)(-iH_\lambda)\psi\,ds$$

We compute

$$\begin{aligned}
&\int_0^h \big(U_\lambda(s)(-iH_\lambda)\psi - U(s)(-iH)\psi\big)\,ds \\
&= \int_0^h U_\lambda(s)(-iH_\lambda + iH)\psi\,ds + \int_0^h (U_\lambda(s) - U(s))(-iH)\psi\,ds.
\end{aligned}$$

With unitarity of $U_\lambda(t)$ we get

$$\left\|\int_0^h \big(U_\lambda(s)(-iH_\lambda)\psi - U(s)(-iH)\psi\big)\,ds\right\| \leq |h|\,\|(-iH_\lambda + iH)\psi\| + \int_0^h \|(U_\lambda(s) - U(s))H\psi\|\,ds.$$

The first term converges to 0 as $\lambda \to \infty$ by (2). The integrand in the second term converges pointwise to 0 as $\lambda \to \infty$ for $s \in [0, h]$. Since

$$\|(U_\lambda(s) - U(s))H\psi\| \leq \|U_\lambda(s)H\psi\| + \|U(s)H\psi\| = 2\,\|H\psi\|$$

holds, we can apply the dominated convergence theorem for Bochner integrals and interchange limit and integral to obtain

$$\frac{U(h)-I}{h}\psi = \lim_{\lambda\to\infty}\frac{1}{h}\int_0^h U_\lambda(s)(-iH_\lambda)\psi\,ds = \frac{1}{h}\int_0^h U(s)(-iH)\psi\,ds$$

Then

$$\lim_{h\to 0}\frac{U(h)-I}{h}\psi = \lim_{h\to 0}\frac{1}{h}\int_0^h U(s)(-iH)\psi\,ds = U(0)(-iH)\psi = -iH\psi$$

Therefore

$$i\frac{d}{dt}\psi(t) = i\lim_{h\to 0}\frac{U(t+h)\psi - U(t)\psi}{h} = iU(t) - iH\psi = U(t)H\psi = HU(t)\psi = H\psi(t)$$

and by definition $\psi(0) = U(0)\psi = \psi$, so $\psi(t)$ is indeed a solution. □

The strongly continuous unitary group $U(t)$ generated by H is denoted by e^{-iHt}. With its help one can make sense of a solution of equation (5.1) for all initial values $\psi \in \mathcal{H}$ even if $\psi \notin \operatorname{dom}(H)$. Theorem (5.4) and (5.8) combined result in the Stone's Theorem which physically translates into the well-defined time evolution of an initial state in the Schrödinger dynamic.

Theorem 5.9 (Stone's Theorem)**.** Every unitary group $(U(t))_{t\in\mathbb{R}}$ on a Hilbert space $\mathcal{H}$ has a unique densely defined, closed generator H, this H is self-adjoint. Conversely, every self-adjoint operator H is the generator of a unique unitary group $(U(t))_{t\in\mathbb{R}}$.

This Theorem delivers the same result as the Hille-Yosida Theorem on Hilbert spaces. Alternatively, it can be proven using the spectral theorem for unbounded operators, see [4, Sec. VIII.4].

6 Hamiltonian of a particle in three dimensions

In this Chapter, we discuss explicit examples that are common and important in the physical context. We start with the Hamiltonian of a free particle which is not contained in a potential. Then, we will prove the famous Kato-Rellich Theorem which gives sufficient conditions for a sum of two operators to be self-adjoint. Using this we are able to extent the first example by adding a bounded potential to the free Hamiltonian. This example will turn out to be rather simple. However, once the potential is unbounded, like in the last part where we cover the Coulomb potential of a hydrogen atom, one has to work a lot harder to get the self-adjointness of the Hamiltonian. For this, we prove the Hardy inequality on the Sobolev space $H^1(\mathbb{R}^3)$.

The underlying Hilbert space is $L^2 := L^2(\mathbb{R}^3)$ with the inner product $\langle f, g\rangle = \displaystyle\int_{\mathbb{R}^3}\overline{f(x)}g(x)\,dx$. $H^2 := H^2(\mathbb{R}^3)$ denotes the Sobolev space of order 2 as defined in the Appendix. All function spaces in this chapter are to be understood in three dimensions even if not explicitly noted.

6.1 Free Hamiltonian

As we have seen in section 2, the Hamiltonian of a free particle in three dimensions is given by

$$H_0 : H^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \quad H_0 = -\Delta = -\sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2} \tag{6.1}$$

where the derivatives are meant in a distributional way as weak derivatives. By our preceding work, it is clear that in order to prove that the time evolution of a quantum system exists and is unique for all initial states $\psi_0 \in \mathcal{H}$, we just need to prove that H_0 is closed, symmetric and lastly self-adjoint.

Theorem 6.1. H_0 is closed.

Proof. Let $(\psi_n)_{n\in\mathbb{N}}$ be a sequence in H^2 with $\psi_n \to \psi$ and $-\Delta\psi_n \to \varphi$ for some $\psi, \varphi \in L^2$. Then the sequence is Cauchy in the graph norm given by $\|\psi_n\|_{H_0} = \|\psi_n\|_{L^2} + \|\Delta\psi_n\|_{L^2}$, which is equivalent to the norm $\|\cdot\|_{H^2}$.
But H^2 is complete, so $\psi_n \to \psi \in H^2$ converges with respect to $\|\cdot\|_{H^2}$. Therefore, $-\Delta\psi_n \to -\Delta\psi$ in L^2 as $n \to \infty$, so $-\Delta\psi = \varphi$. $\square$

Theorem 6.2. H_0 is symmetric.

Proof. For all $\psi, \varphi \in C_c^\infty$ we have

$$\langle \psi, H_0\varphi \rangle = \int_{\mathbb{R}^3} \overline{\psi(x)}(-\Delta\varphi)(x)\ dx = \int_{\mathbb{R}^3} \overline{(-\Delta\psi)(x)}\varphi(x)\ dx = \langle H_0\psi, \varphi \rangle$$

by integration by parts, where the boundary terms vanish since the functions have compact support. The same holds for $\psi, \varphi \in H^2$ since C_c^∞ is dense in H^2 with respect to $\|\cdot\|_{L^2}$. Let $\psi, \varphi \in H^2$. We choose $(\psi_n)_{n\in\mathbb{N}}, (\varphi_n)_{n\in\mathbb{N}} \subseteq C_c^\infty$ such that $\psi_n \to \psi$, $\varphi_n \to \varphi$ in H^2. Therefore, we have

$$H_0\psi_n = -\Delta\psi_n \to -\Delta\psi = H_0\psi \text{ as } n \to \infty \tag{6.2}$$

and the same for φ. With the continuity of the inner product we get

$$\begin{aligned} \langle \psi, H_0\varphi \rangle &\overset{(6.2)}{=} \left\langle \lim_{n\to\infty} \psi_n, \lim_{m\to\infty} H_0\varphi_m \right\rangle = \lim_{n\to\infty} \lim_{m\to\infty} \langle \psi_n, H_0\varphi_m \rangle = \lim_{n\to\infty} \lim_{m\to\infty} \langle H_0\psi_n, \varphi_m \rangle \\ &\overset{(6.2)}{=} \langle H_0\psi, \varphi \rangle . \end{aligned}$$

Therefore, $H_0 = -\Delta$ is symmetric on H^2. $\square$

We can determine the spectrum of $H_0 = -\Delta$ to prove self-adjointness, this is done by using the Fourier transformation. For more details, compare [7, Ex. 8.1].

Theorem 6.3. H_0 is self-adjoint.

Proof. By Theorem (6.2) H_0 is symmetric, so we can use Theorem (3.8). We denote the Fourier transformation and its inverse by $\mathcal{F}$ and $\mathcal{F}^{-1}$ respectively, as defined in the Appendix.
Then $\mathcal{F}(-\Delta f)(\xi) = |\xi|^2 \hat{f}(\xi)$, so we can rewrite the Laplacian as $-\Delta = \mathcal{F}^{-1} |\xi|^2 \mathcal{F}$ where $|\xi|^2$ is a multiplication operator in the Fourier space. Here it is crucial, that the domain of $-\Delta$ is H^2, since this is exactly where this transformation is allowed.
Hence, $z - (-\Delta) = \mathcal{F}^{-1} z \mathcal{F} - \mathcal{F}^{-1} |\xi|^2 \mathcal{F} = \mathcal{F}^{-1}(z - |\xi|^2)\mathcal{F} \implies z - (-\Delta)$ is of bounded inverse if and only if $z - |\xi|^2$ is invertible for all $\xi \in \mathbb{R}^3$. This is the case for $z \notin [0, \infty)$, so $\rho(H_0) = \rho(-\Delta) = \mathbb{C} \setminus [0, \infty)$. Therefore $\sigma(H_0) = \sigma(-\Delta) = [0, \infty)$. By Theorem (3.10) $H_0 = -\Delta$ is self-adjoint. $\square$

6.2 Kato-Rellich Theorem

In physics, oftentimes a particle is not free but exposed to some potential. In order to study the time evolution of such systems, we are interested in the self-adjointness of the operator $-\Delta + V$, where $V(x)$ is a potential dependent on the spherical coordinates acting as a multiplication operator. Therefore, we want to find a criterion for the self-adjointness of a sum of two operators. The following result is the famous Kato-Rellich-Theorem, [8, Sec. X.2, Thm X.12]. A more general version can be found in [7, Thm 8.5].

Theorem 6.4 (Kato-Rellich)**.**
Let $A : \mathrm{dom}(A) \to \mathcal{H}$ be a self-adjoint operator and $B : \mathrm{dom}(B) \to \mathcal{H}$ symmetric with $\mathrm{dom}(A) \subseteq \mathrm{dom}(B) \subseteq \mathcal{H}$.
If there exist $a, b \in \mathbb{R}$ with $a < 1$ such that for all $\varphi \in \mathrm{dom}(A) : \|B\varphi\| \leq a \|A\varphi\| + b \|\varphi\|$, then $A + B : \mathrm{dom}(A) \to \mathcal{H}$ is self-adjoint.

Proof. Clearly, $A+B$ is symmetric on $\mathrm{dom}(A)$ by the linearity of the inner product. By Theorem (3.8), it is enough to prove $\mathrm{ran}(A+B+i\mu) = \mathcal{H}$ for $\mu \in \mathbb{R}\setminus\{0\}$ with $|\mu|$ large enough. By Lemma (3.10), $-i\mu \in \rho(A)$, so $A + i\mu$ is invertible and $A + B + i\mu = (I + B(A + i\mu)^{-1})(A + i\mu)$. We will show that $\left\|B(A + i\mu)^{-1}\right\| < 1$ for $|\mu|$ large enough. If this holds, then Lemma (3.1) implies that $I + B(A + i\mu)^{-1} : \mathcal{H} \to \mathcal{H}$ is of bounded inverse. A is self-adjoint, hence $\mathrm{ran}(A + i\mu) = \mathcal{H}$ and $(A + i\mu)^{-1}$ is bounded. Then

$$(A + B + i\mu)^{-1} = (A + i\mu)^{-1}(I + B(A + i\mu)^{-1})^{-1}$$

exists and is bounded as desired. Let $\varphi \in \mathcal{H}$ and set $\psi := (A + i\mu)^{-1}\varphi \in \mathrm{dom}(A)$. Then $\left\|B(A + i\mu)^{-1}\varphi\right\| = \|B\psi\| \leq a \|A\psi\| + b \|\psi\|$. Furthermore, for suitable $\mu \in \mathbb{R} \setminus \{0\}$:

$$\|A\psi\| \leq \|(A + i\mu)\psi\| = \|\varphi\| \text{ and } \|\varphi\| = \|(A + i\mu)\psi\| \geq |\mu| \|\psi\| \qquad \implies \|\psi\| \leq \frac{\|\varphi\|}{|\mu|}$$

Combining the inequalities, we get

$$\left\|B(A + i\mu)^{-1})\varphi\right\| \leq a \|\varphi\| + \frac{b}{|\mu|} \|\varphi\| \leq \left(a + \frac{b}{|\mu|}\right) \|\varphi\| \quad \text{for all } \varphi \in \mathcal{H}$$

Thus, $\left\|B(A + i\mu)^{-1}\right\| \leq a + \frac{b}{|\mu|}$ and since $a < 1$ by assumption, choosing $|\mu|$ large enough we obtain $\left\|B(A + i\mu)^{-1}\right\| < 1$. $\square$

6.3 Hamiltonian with bounded potential

Firstly, we consider a bounded potential $V \in L^\infty(\mathbb{R}^3)$, then the domain of the corresponding multiplication operator $\operatorname{dom}(V)$ is the whole Hilbert space. The Hamiltonian takes on the form $H = H_0 + V : H^2 \to L^2$.
A very common application of such a potential is the quantum well, where a particle is contained in a spatially restricted, constant potential: $V(x) = \begin{cases} -V_0 & \text{for } |x| < a \\ 0 & \text{else} \end{cases}$ for some $a > 0$.

Theorem 6.5. $H = -\Delta + V$ is self-adjoint.

Proof. $-\Delta$ is self-adjoint by Theorem (6.3). First, we prove that V is symmetric by using that $V(x)$ is real for all $x \in \mathbb{R}^3$. For all $\psi, \varphi \in L^2$ we have:

$$\langle \psi, V\varphi \rangle = \int \overline{\psi(x)}(V\varphi)(x)\, dx = \int \overline{\psi(x)} V(x)\varphi(x)\, dx = \int \overline{V(x)\psi(x)}\varphi(x)\, dx = \langle V\psi, \varphi \rangle$$

Since $V \in L^\infty$ we have $C := \|V\|_\infty = \sup_{x\in\mathbb{R}^3} |V(x)| < \infty$. Therefore,

$$\|V\psi\|^2 = \int |V(x)|^2 |\psi(x)|^2\, dx \le C^2 \int |\psi(x)|^2\, dx = C^2 \|\psi\|^2 \implies \|V\psi\| \le C\|\psi\|$$

By Theorem (6.4) the operator $-\Delta + V : H^2 \to L^2$ is self-adjoint. $\square$

6.4 Hamiltonian with Coulomb potential

The Coulomb potential of a hydrogen atom is given by $V : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R},\ V(x) = -\frac{1}{|x|}$ with a singularity at the origin $x = 0$. We extend it to $V : \mathbb{R}^3 \to \mathbb{R},\ V(x) = \begin{cases} -\frac{1}{|x|} & \text{for } x \neq 0 \\ 0 & \text{for } x = 0 \end{cases}$.
With the following inequality we see that the domain of the linear multiplication operator V contains H^2.

Theorem 6.6 (Hardy inequality)**.** For all $\psi \in H^1(\mathbb{R}^3)$:

$$\int \frac{|\psi(x)|^2}{|x|^2}\, dx \le 4 \int |\nabla\psi(x)|^2\, dx \tag{6.3}$$

Proof. First assume $\psi \in C_c^\infty$, then we have

$$\sum_{i=1}^{3} \int \left(\partial_i \frac{x_i}{|x|^2}\right) |\psi(x)|^2\, dx = \sum_{i=1}^{3} \left[\int \frac{|\psi(x)|^2}{|x|^2}\, dx + \int \frac{x_i(-\partial_i |x|^2)}{|x|^4} |\psi(x)|^2\, dx\right]$$

$$= \sum_{i=1}^{3} \left[\int \frac{|\psi(x)|^2}{|x|^2}\, dx - \int \frac{2x_i^2}{|x|^4} |\psi(x)|^2\, dx\right] = 3\int \frac{|\psi(x)|^2}{|x|^2}\, dx - 2\int \frac{|\psi(x)|^2}{|x|^2}\, dx.$$

Thus,

$$\int \frac{|\psi(x)|^2}{|x|^2}\, dx = \sum_{i=1}^{3} \int \left(\partial_i \frac{x_i}{|x|^2}\right) |\psi(x)|^2\, dx = -\int \sum_{i=1}^{3} \frac{x_i}{|x|^2} \partial_i |\psi(x)|^2\, dx$$

applying integration by parts where the boundary terms vanish since ψ has compact support. Taking the absolute value, we get

$$\int \frac{|\psi(x)|^2}{|x|^2}\,dx = -\int \sum_{i=1}^{3} \frac{x_i}{|x|^2}\, 2\,\mathrm{Re}\big(\overline{\psi(x)}\partial_i\psi(x)\big)\,dx \le 2\int \frac{\left|\overline{\psi(x)}\right|}{|x|}\frac{\left|\sum_{i=1}^{3} x_i\partial_i\psi(x)\right|}{|x|}\,dx$$

$$\le 2\int \frac{|\psi(x)|}{|x|}\frac{|\langle x, \nabla\psi(x)\rangle|}{|x|}\,dx \le 2\int \frac{|\psi(x)|}{|x|}\,|\nabla\psi(x)|\,dx$$

where we used Cauchy-Schwarz in the last equation. Using it again, we obtain

$$\int \frac{|\psi(x)|^2}{|x|^2}dx \le 2\Big(\int \frac{|\psi(x)|^2}{|x|^2}dx\Big)^{\frac{1}{2}} \Big(\int |\nabla\psi(x)|^2\,dx\Big)^{\frac{1}{2}}.$$

This implies equation (6.3) for all $\psi \in C_c^\infty$. Assume now that $\psi \in H^1$. Since C_c^∞ is dense is H^1 w.r.t. $\|\cdot\|_{H^1}$, there is a sequence $(\psi_n)_{n\in\mathbb{N}}$ in C_c^∞ with $\psi_n \to \psi$ in H^1 as $n \to \infty$, so $\psi_n \to \psi$ and $\partial_i\psi_n \to \partial_i\psi$ in L^2. Then there is a subsequence $(\psi_{n_k})_{k\in\mathbb{N}}$ with $\psi_{n_k} \to \psi$ as $k \to \infty$ almost everywhere. The Hardy inequality applies to all $\psi_{n_k} \in C_c^\infty$, then Fatou's Lemma gives

$$\int \frac{|\psi(x)|^2}{|x|^2}\,dx \le \liminf_{k\to\infty}\int \frac{|\psi_{n_k}(x)|^2}{|x|^2}\,dx \le 4\int |\nabla\psi(x)|^2\,dx$$

as desired. This proves the equation (6.3) for all $\psi \in H^1(\mathbb{R}^3)$. □

For more general forms of this inequality, see [9, On the Hardy–Sobolev Inequalities].

Applying the Hardy inequality to $\psi \in H^2$ we get

$$\|V\psi\|^2 = \int \frac{|\psi(x)|^2}{|x|^2}\,dx \le 4\int |\nabla\psi(x)|^2\,dx < \infty,$$

so $\psi \in \mathrm{dom}(V)$. Therefore, the Coulomb Hamiltonian $H_C = H_0 + V : H^2 \to L^2$ is well-defined on H^2.

Theorem 6.7. *$H_C = -\Delta + V$ is self-adjoint.*

Proof. $-\Delta$ is self-adjoint by Theorem (6.3). For all $\psi \in H^2(\mathbb{R}^3) \subseteq H^1(\mathbb{R}^3)$ the Hardy inequality reads

$$\|V\psi\|^2 = \int \frac{|\psi(x)|^2}{|x|^2}\,dx \le 4\int |\nabla\psi(x)|^2\,dx.$$

Let $\varepsilon > 0$. The Plancherel Identity, [8, Sec. 2.2], gives

$$\int |\nabla\psi(x)|^2\,dx = \|\nabla\psi\|^2 = \|\mathcal{F}(\nabla\psi)\|^2 = \int \left|\xi\hat{\psi}(\xi)\right|^2 d\xi = \int \xi^2\left|\hat{\psi}(\xi)\right|^2 d\xi.$$

We have $\left(\varepsilon\xi^2 - \frac{1}{2\varepsilon}\right)^2 \ge 0$, so $\xi^2 \le \varepsilon^2\xi^4 + \frac{1}{4\varepsilon^2}$ and

$$\int \xi^2\left|\hat{\psi}(\xi)\right|^2 d\xi \le \varepsilon^2\int \xi^4\left|\hat{\psi}(\xi)\right|^2 d\xi + \frac{1}{4\varepsilon^2}\int \xi^4\left|\hat{\psi}(\xi)\right|^2 d\xi = \varepsilon^2\,\|-\Delta\psi\|^2 + \frac{1}{4\varepsilon^2}\,\|\psi\|^2$$

$$\le \left(\varepsilon\,\|-\Delta\psi\| + \frac{1}{2\varepsilon}\,\|\psi\|\right)^2 < \infty.$$

Hence, the norm $\|V\psi\| \leq \varepsilon \|-\Delta\psi\| + \frac{1}{2\varepsilon}\|\psi\|$ is finite for $\psi \in H^2(\mathbb{R}^3)$. Thus, for all $\psi \in H^2(\mathbb{R}^3)$ we get $V\psi \in L^2(\mathbb{R}^3)$ and $\|V\psi\| \leq \varepsilon \|-\Delta\psi\| + \frac{1}{2\varepsilon}\|\psi\|$. Choosing $\varepsilon < 1$, by Theorem (6.4) the operator $-\Delta + V : H^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is self-adjoint. $\square$

7 Outlook

In this thesis, we were able to prove that there exists a unique solution for each initial value in the domain of the Hamiltonian if and only if it is self-adjoint on this domain.
Now that we can control the Schrödinger equation for a self-adjoint H which is constant in time, the next step can be to consider a time-dependent Hamiltonian operator $H(t)$.
This can be done via perturbation theory. Assume $H = H_0 + V(t)$ where H_0 is a time-independent Hamiltonian. In the absence of a perturbation we obtain the unique time evolution $U_0(t)$, see Stone's Theorem (5.9). We define the time evolution for an arbitrary starting point $t_0 \neq 0$ as $U_0(t, t_0) := U_0(t - t_0) = U_0(t)U_0(-t_0)$.
Fix $t, t_0 \in \mathbb{R}$. The goal is to obtain an evolution $U(t, t_0)$ for the time-dependent Hamiltonian H. By differentiating $U_0(t_0, t)U(t, t_0)$ one derives that the Hamiltonian H yields a time evolution described by the Volterra equation:

$$U(t, t_0) = U_0(t) - i \int_{t_0}^{t} U_0(t, s)V(s)U(s, t_0)\, ds$$

Now consider a bounded potential $V(t)$ with $\|V(t')\| \leq C$ for all $t' \in [0, t]$. The equation can be solved iteratively by plugging $U(t, t_0)$ into itself to obtain the Neumann series:

$$U(t, t_0) = \sum_{n=0}^{\infty} (-i)^n \int_{t_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2 \cdots \int_{t_0}^{s_{n-1}} ds_n\, U_0(t, s_1)V(s_1)U_0(s_1, s_2)V(s_2) \dots U_0(s_n, t_0) \tag{7.1}$$

We already know that $U_0(t)$ is unitary, so $\|U_0(t_1, t_2)\| \leq 1$ for all $t_1, t_2 \in \mathbb{R}$. Hence, the sum converges absolutely in operator norm:

$$\begin{aligned}\|U(t, t_0)\| &\leq \sum_{n=0}^{\infty} \int_{t_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2 \cdots \int_{t_0}^{s_{n-1}} ds_n\, \|U_0(t, s_1)V(s_1)U_0(s_1, s_2)V(s_2) \dots U_0(s_n, t_0)\| \\ &\leq \sum_{n=0}^{\infty} \int_{t_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2 \cdots \int_{t_0}^{s_{n-1}} ds_n\, C^n = \sum_{n=0}^{\infty} \frac{1}{n!} C^n (t - t_0)^n = e^{C(t - t_0)} < \infty\end{aligned}$$

One can show that the converging series in 7.1 does in fact deliver the correct time evolution for H.
However, if V is not bounded, the series does not necessarily converge and we must find another way to approximate $U(t, t_0)$. Considering how much work has gone into finding $U_0(t)$ for a fairly nice self-adjoint time-independent Hamiltonian, this may turn out to be rather complicated and for certain choices of H and $V(t)$, are still very much a topic of current research.

8 Appendix

We introduce some basic function spaces and their properties.

Definition 8.1. Space of smooth functions with compact support:
$C_c^\infty(\mathbb{R}^n) := \{\phi : \mathbb{R}^n \to \mathbb{C} \,|\, \phi \in C^\infty \text{ and } \operatorname{supp}(\phi) \text{ is compact}\}$ with $\operatorname{supp}(\phi) = \overline{\{x \in \mathbb{R}^n \,|\, \phi(x) \neq 0\}}$

Definition 8.2. $L^p(\mathbb{R}^n) := \left\{\phi : \mathbb{R}^n \to \mathbb{C} \,|\, \int_{\mathbb{R}^n} \|\phi(x)\|^p \, dx < \infty\right\}$

Fact 8.1. $L^p(\mathbb{R}^n)$ is a Banach space when equipped with the norm

$$\|f\|_{L^p} := \left(\int_{\mathbb{R}^n} |f(x)|^p \; dx\right)^{\frac{1}{p}}$$

[4, Thm III.1 (b) (Riesz-Fisher)]

Definition 8.3. Multiindex $\alpha = (\alpha_1, \dots, \alpha_n) \;\to \partial^\alpha = \partial_{x_1}^{\alpha_1} \dots \partial_{x_n}^{\alpha_n}$ and $|\alpha| = \alpha_1 + \dots \alpha_n$

$\partial^\alpha u$ denotes the weak derivative, which is defined as the unique function ω that satisfies

$$\forall \phi \in C_c^\infty(\mathbb{R}^n) : \int_{\mathbb{R}^n} u \partial^\alpha \phi \; dx = (-1)^{|\alpha|} \int_{\mathbb{R}^n} \omega \phi \; dx$$

Definition 8.4. Sobolev space of order k:

$$H^k(\mathbb{R}^n) := \left\{u \in L^2(\mathbb{R}^n) \,|\, \partial^\alpha u \in L^2(\mathbb{R}^n) \text{ for all } \alpha \text{ with } |\alpha| \leq k\right\} \subseteq L^2(\mathbb{R}^n) \tag{8.1}$$

equipped with the inner product

$$\langle f_1, f_2 \rangle := \int_{\mathbb{R}^d} \overline{\hat{f}_1(\xi)} \hat{f}_2(\xi)(1 + |\xi|^2)^k \; d\xi \tag{8.2}$$

where the overline denotes the complex conjugation and $\hat{f}$ denotes the Fourier transformation on L^2.
H^k is a Banach space with the norm $\|u\| = \left(\left\|\sum_{|\alpha| \leq k} (\partial^\alpha u)\right\|_{L^2}^2\right)^{\frac{1}{2}}$, which is equivalent to the norm induced by the inner product.

We have $C_c^\infty(\mathbb{R}^n) \subseteq H^2(\mathbb{R}^n) \subseteq H^1(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^3)$.

Theorem 8.1 (Embeddings)**.**

1. $C_c^\infty(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$ w.r.t. $\|\cdot\|_{L^2}$

   Therefore, $H^2(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$ w.r.t. $\|\cdot\|_{L^2}$.
2. $C_c^\infty(\mathbb{R}^n)$ is dense in $H^1(\mathbb{R}^n)$ w.r.t. $\|\cdot\|_{H^1}$

For more on this, see [1] and [10].

Definition 8.5. We denote the space of bounded and linear operators on a Banach space X as $\mathrm{BL}(X)$ with the operator norm

$$\|A\| = \sup_{x \in X} \frac{\|Ax\|}{\|x\|}. \tag{8.3}$$

Then for all $x \in X$: $\|Ax\| \leq \|A\| \, \|x\|$. By [4, Thm III.2] $\mathrm{BL}(X)$ is a Banach space.
We call a linear operator A bounded if $\|A\| < \infty$. This is equivalent to A being continuous, see [4, Thm I.6].

Lemma 8.2 (Fourier Transformation)**.** Let $\mathcal{F}$ denote the Fourier Transformation on $L^2(\mathbb{R}^n)$. It is defined as the unique continuous mapping $\mathcal{F} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ that extends the mapping $F : \mathcal{S} \to L^2(\mathbb{R}^n)$, where $\mathcal{S}$ is the Schwartz class. Further information can be found in [8, Sec. IX.1].
For $f \in L^2(\mathbb{R}^n)$ the Plancherel identity, [8, Thm IX.1 Corollary], holds:

$$\int_{\mathbb{R}^n} |f(x)|^2 \, dx = \int_{\mathbb{R}^n} |\mathcal{F}f(x)|^2 \, dx$$

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Eigenständigkeitserklärung

Hiermit erkläre ich, die vorliegende Arbeit selbstständig verfasst zu haben und keine anderen als die in der Arbeit angegebenen Quellen und Hilfsmittel benutzt zu haben.

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