Distributions, Fourier Analysis and Quantum Mechanics

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1 Introduction

What is an atom?

Between 1909 and 1913, a group of physicists (Rutherford, von den Broeck indenpendently Bohr) sought to describe atoms with a model. Due to many successful experiments with radiation, it was apparent that protons and neutrons must sit inside the core of the atom (the *nucleus*), whereas electrons somehow circle more flexibly outside, arranged in layers. Their view on atoms, which shaped the periodic table of elements, was as follows

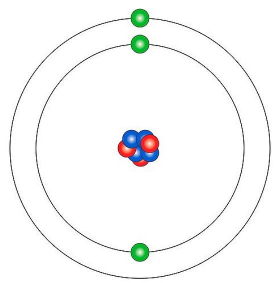

Figure 1: Atomic structure of Lithium. Protons are red, neutrons are blue and electrons are green

This model was very good at explaining many phenomena in physics and chemistry. But there is a fundamental question:

- **Question.** Why do the (negatively charged) electrons not crash into the (positively charged) nucleus?

This is against all odds, since we do know that different charges attract each other via a *Coulomb force*. How to deal with this? A suspicion that can easily arise is that it is maybe incorrect to look at electrons/protons/neutrons as *particles*. But what other objects are there? One object that was quite a bit understood at this time were *waves*, due to many experiments with light.

Particles or Waves?

But why should electrons be waves? Well, the wave property could at least explain the organization in layers! Imagine you have a string of a guitar. This string is usually clamped on both sides. Now you pull the string. What you observe is that the signal is composed of *elementary waves*, that is waves whose wavelength is $\frac{1}{n}$-times the total length of the string for $n \in \mathbb{N}$. For $n = 1$ this wave is called *base wave*, for $n = 2$ this is the *first overtone wave* etc etc. An observation that is important for the whole theory of quantum mechanics is that all these waves have *different energy levels*. This distunguishes the elementary waves and shows that their energy is *quantized* (i.e. located on discrete levels).

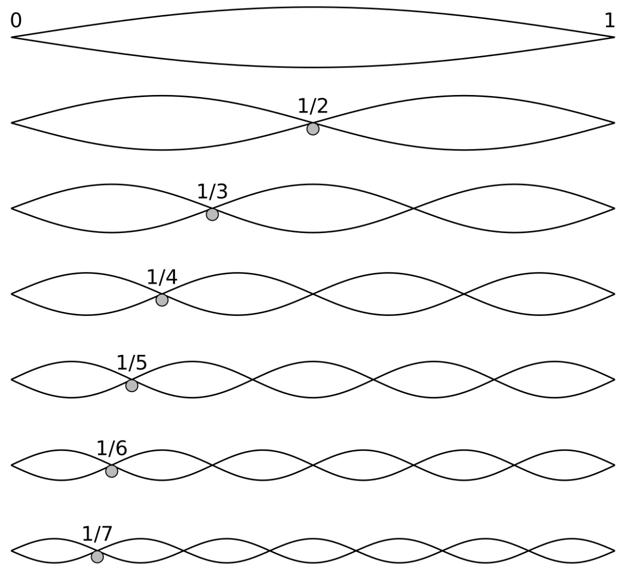

Figure 2: Base wave and overtones.

Now back to our atom: Imagine now one end of a string is sitting inside the center nucleus and one end is located at the "outside end" of the atom (if this at all exists). If an electron were sitting inside the center of the nucleus it cannot move due to the charges there. At the "outside end" it also shouldn't move (since it shouldn't escape). What we have is exactly the situation of our guitar string that is clamped at two ends. And as a result, we must observe quantized energy levels. This accounts for the layers in which the electrons are arranged – and is a strong hint towards the fact that electrons behave like waves

The double slit experiment

Between 1923 and 1927 the physiciststs C. Davisson and L. Germer wanted to know for sure. Are electrons really waves? To understand this they have set up an experiment that was expected to clear up the situation once and for all (instead new questions arouse from it...). A similar experiment has also already successfully explained the wave nature of visible light. It goes as follows: An electron beam gun shoot one electron after each other on a wall with to very narrow slits. Some distance behind this wall there is a detector screen that can detect where the electrons hit the screen level.
Now, if electrons are particles, they just decide for one of the slits and then they can hit the detector screen just directly behind the two slits. On contrary, if they are waves it will happen that from each of the two slits there originates a new wave. These two waves will

then interact with each other and form an *interference pattern*, which will become visible at the detector screen.

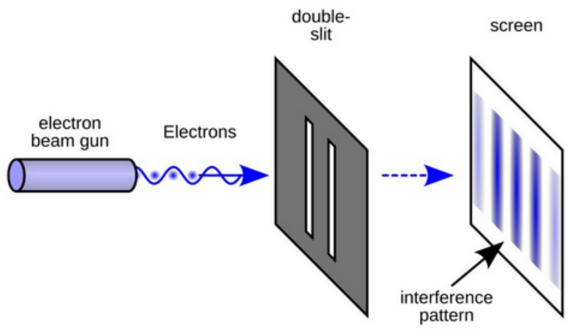

Figure 3: Double slit experiment

Now, what happened in the experiment? The interference pattern was observed. There was however one more experiment conducted, which led to more confusion. Instead of detecting the electron only at the detector screen, it was also detected at one of the slits, whether the electron goes through this slit or not. And a big surprise happened: If such an additional detector is installed, then suddenly the electrons behave like particles (no matter which slit they actually go through). This is really confusing: detection changes how the system behaves. And this gives rise to a few insights that form the basis of our description

- Electrons (and other subatomic particles) can be both —*particles and waves*!
- Since in a quantum system everything interacts with each other and even measurements change the system, it is impossible to describe positions without uncertainty.

These facts must be taken into account when formulating quantum mechanics. In particular: All the statements should be *probabilistic statements*.

How to formulate quantum mechanics?

Here we allow ourselves to be mathematically very sloppy, in the next chapter we will be much more rigorous (which is basically the purpose of this lecture). Let us look at a quantum system, e.g. some electron in the d-dimensional space $\mathbb{R}^d$ that moves over time. We introduce a (time-and-space-dependent) *state function*

$$\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}, \psi = \psi(t,x), \quad \text{such that} \quad \int_{\mathbb{R}^d} |\psi(t,x)|^2 \, \mathrm{d}x = 1. \tag{1}$$

This function ψ enables us to make the probabilitstic statements above in the following sense: For all $J \subset \mathbb{R}^d$ (suitably nice) we can say

$$\mathbb{P}[\text{The electron is inside the set } J \text{ at time } t] = \int_J |\psi(t,x)|^2 \, \mathrm{d}x,$$

where $\mathbb{P}[\cdot]$ stands for the probability of an event. Hence we have a *probablility distribution* for the position of the particle. Its (time-dependent) *probability density* is given by $|\psi(t,\cdot)|^2$. Now that we have this probability density given we can use it, e.g. to form *expected values.* With this we should be able to assign some *expected trajectory* to the electron. We specialize on the case $d = 1$ to make this easier to see. The place of the electron at time t can be looked at as a random variable. Since we know its probability density $|\psi(t,\cdot)|^2$, its expected value can be expressed as

$$\mathbb{E}[\text{Position of the electron at time } t] = \int_{\mathbb{R}} x \cdot |\psi(t,x)|^2 \, \mathrm{d}x,$$

(at least if this integral exists). Physical properties of a system are best destribed if one has both: position and velocity (or better: momentum). The latter one is also a random variable. It will turn out that

$$\mathbb{E}[\text{Momentum of the electron at time } t] = \int_{\mathbb{R}} x \cdot |\hat{\psi}(t,x)|^2 \, \mathrm{d}x,$$

where $\hat{\psi}(t,\cdot)$ is the Fourier transform of $\psi(t,\cdot)$. We will give a mathematical explanation why for the momentum we have to take the Fourier transform here (much based on the fact that the Fourier transform transforms derivatives, i.e. taking velocities, into multiplications). Guided by this observation, we will understand that the momentum can be looked at as a random variable with probability density $|\hat{\psi}(t,\cdot)|^2$. Note that this is indeed a probability density since a property of the Fourier transform (more precisely, its unitariness) implies

$$\int_{\mathbb{R}} |\hat{\psi}(t,x)|^2 \, \mathrm{d}x = \int_{\mathbb{R}} |\psi(t,x)|^2 \, \mathrm{d}x = 1.$$

Agenda

Now that we fixed the formulation, let me give you a list of goals we have in this course

1. **Heisenberg's Uncertainty Principle.** We have discussed the random variables *position* and *momentum*. In classical mechanics, both are things that we can measure and therefore they are always deterministic and never really random. In quantum mechanics, I can never know them both. More precisely, the *variances* of these random variables satisfy
$$\mathbb{VAR}[\text{Position}] \cdot \mathbb{VAR}[\text{Momentum}] \geqslant \frac{h^2}{16\pi^2},$$
where h is a natural constant. This inequality holds regardless of the precise state function ψ and in particular for all times throughout the entire lifetime of the system. This shows also: If we detect the position of a particle we must necessarily have a lot of uncertainty in the momentum. Hence our position measurements will never describe the system completely.

2. **Schrödinger equation.** In the above experiments we have discussed a few quantum systems, both times with an electron involved. To be able to describe them thoroughly,

we need to find an equation that describes the dynamics of these electrons. This is done by means the *Schrödinger equation*, which describes the evolution of the state function of an electron which is located in a (time-independent) potential $V : \mathbb{R}^d \to \mathbb{R}, V = V(x)$. More precisely, If ψ is the state function of the system, we would like to say that for all $(t, x) \in \mathbb{R} \times \mathbb{R}^d$

$$i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2}\Delta_x\psi(t,x) + V(x)\psi(t,x), \quad \text{where } \Delta_x = \sum_{i=1}^{d}\frac{\partial^2}{\partial x_i^2}. \tag{2}$$

Mathematicians might notice some flaws here: We want to take derivatives of ψ, but all we required on ψ in (1) is square integrability – in particular differentiability is not for granted. Luckily, we have the concept of *distributions*, which allows us to assign derivatives to non-differentiable functions. Hence, we will look at ψ as a distribution and not a function anymore. While this seems like a suitable approach here, it creates another problem: While differentiating a distribution is easy, multiplying a distribution with a function is not. So the last summand on the right hand side of (2) deserves some more attention.

(a) **The free propagator, $V = 0$.** We will first ignore the issue of multiplying functions and distributions, by assuming that the potential term is absent, i.e. $V = 0$. This is already sufficient to describe the double slit experiment as there no potential is present. Our main result will be as follows. If a state function ψ satisfies (in a yet to be discussed distributional sense) (2), and the initial state function is $\psi(0,\cdot) := \psi_0$ then (under mild regularity assumptions on ψ_0) we have

$$\psi(t,x) = \int_{\mathbb{R}^d}\frac{1}{(2\pi i t)^{\frac{d}{2}}}e^{i\frac{|x-y|^2}{2t}}\psi_0(y)\,\mathrm{d}y.$$

That means that we can compute the complete evolution explicitly if we have given just the initial state. The function $P_0(t,x,y) := \frac{1}{(2\pi i t)^{\frac{d}{2}}}e^{i\frac{|x-y|^2}{2t}}$ that allows this explicit computation is called the *free propagator*. Having this at hand we can describe, why the interference pattern appears in the double slit experiment.

(b) **Propagators with Potentials.** We turn again to the atom model. Here the electrons are inside a force field, determined by the *Coulomb atttraction force* that comes from the protons (which we assume to be located at the origin). In particular, the nucleus at the origin creates a *Coulomb potential* given by $V(x) = \frac{c}{4\pi\varepsilon_0|x|}$ (where c is the number of protons at the origin). We would like to solve (2) with this potential. What does *solve* mean here? We would like to have as in case (a) a *propagator* $U(t,x,y)$ depending on V with the property that

$$\psi(0,\cdot) = \psi_0 \qquad \Longrightarrow \qquad \psi(t,x) = \int_{\mathbb{R}^d}U(t,x,y)\psi_0(y)\,\mathrm{d}y,$$

i.e. $U(t,x,y)$ permits computation of $\psi(t,\cdot)$ given the initial state ψ_0. Using some functional analysis we are able formulate a condition for such a propagator to exist. The main result is that such a propagator exists if and only if

$$-\frac{1}{2}\Delta_x + V\mathrm{Id} : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C}) \qquad \text{is a self-adjoint operator.}$$

We will define later rigorously what a self-adjoint operator is. At this point let me express a caveat: In physics literature, quantum mechanics is usually happening on some finite-dimensional Hilbert space $\mathbb{C}^n$. For an operator $A : \mathbb{C}^n \to \mathbb{C}^n, x \mapsto Mx$ (where $M \in \mathbb{C}^{n\times n}$ is a matrix), it is known from linear algebra what it means to be self-adjoint: Namely, $\overline{M}^T = M$. This is easy to verify. However, in infinite dimensional spaces there is much more to explain about the notion of self-adjointness – even the definition of it can fill pages in some literature. And not just that: This notion of self-adjointness will necessitate regularity requirements on V that could not be identified by reducing quantum mechanics to the finite-dimensional setting. Luckily, at least our Coulomb potential satisfies these requirements. Finally, we will be able to compute the desired propagator (asymptotically) by means of *Trotter's product Formula.* This is mathematically what physicists call a *path integral.*

(c) **Spectral Theory and Stone's Theorem.** The fact that a propagator exists for self-adjoint operators is mathematically based on spectral threory for self-adjoint operators. If time allows we will discuss some foundations of this theory.

Literature

- Erwin Kreyszig. *Introductory Functional Analysis with Applications* (1978).
  - Chapter 11.1/11.2 forms the basis of our Chapter 2.
  - In general Chapter 11 is a good read with a lot of detailed explanations of physics. For us however pursuing it further is not ideal: It focuses much on the Time-Independent Schrödinger equation. While this is very interesting, it would not fit to the background of this course coming Distribution Theory and Fourier Analysis.
- Michael Reed and Barry Simon. Methods of Modern Mathematical Physics. Part I: Functional Analysis.
  - From this book's Chapter VIII.8, Chapter 3.3.1 and 3.3.2 are taken
  - It is a self-contained introduction into Functional Analysis and contains theory about unbounded operators.
- Michael Reed and Barry Simon. Methods of Modern Mathematical Physics. Part II: Fourier Analysis and Self-Adjointness
  - This book is a general guide through the covered material. After the whole lecture, you should have covered Chapter IX.1-IX.7 and Chapter X.1-2 and X.11.
- Stefan Teufel. Mathematical Quantum Theory. Winter Term 2020/2021

- Chapters 3.1 and 3.2 are partially based on these lecture notes
- These lecture notes are very well-structured and contain eveything that is needed for matheamtical quantum mechanics. Since the lecture notes have more of a supplementary character, some explanations / details are missing at times.

- Marius Müller. *Analysis III* (2024)
  - I will often reference some results from these lecture notes which are publicly available at `https://www.uni-augsburg.de/de/fakultaet/mntf/math/einricht/ik/` (Click "Skripte")

2 Foundations of Quantum mechanics

08.06.2026

To motivate quantum mechanics, let us consider the simplest case of a physical system: a single particle on the real line $\mathbb{R}$. In classical mechanics, the state of our system at some instant is described by specifying position and velocity of the particle. So, two numbers describe the state of the particle. In quantum theory, describing a particle is more complicated – the quantities named above are not deterministic (since observing what a particle does change the system). Instead, we want to make probabilistic statements about the system. To this end we introduce a *state function* $\psi \in L^2(\mathbb{R};\mathbb{C})$ which satisfies

$$\int_{\mathbb{R}} |\psi(x)|^2 \, \mathrm{d}x = 1.$$

Here, $\mathrm{d}x$ indicates integration with respect to the 1-D Lebesgue measure. The probability that the particle is then found in a given Lebesgue-measurable subset $J \subseteq \mathbb{R}$ is then given by

$$\mathbb{P}_\psi[J] := \int_J |\psi(x)|^2 \, \mathrm{d}x.$$

One readily checks that $\mathbb{P}_\psi$ is then a probability distribution with density $x \mapsto |\psi(x)|^2$. In order to describe this probability distribution, we can define known probabilistic quantities like the *expected value*

$$\mu_\psi := \int_{\mathbb{R}} x|\psi(x)|^2 \, \mathrm{d}x \tag{3}$$

and the *variance*

$$\mathrm{var}_\psi := \int_{\mathbb{R}} (x-\mu_\psi)^2|\psi(x)|^2 \, \mathrm{d}x \tag{4}$$

Notice that due to (3) μ_ψ can be written as

$$\mu_\psi = \int_{\mathbb{R}} x\psi(x)\overline{\psi(x)} \, \mathrm{d}x. \tag{5}$$

For the formulation of the theory, it is helpful to express all the quantities we consider by means of the *scalar product*

$$\langle \cdot,\cdot \rangle : L^2(\mathbb{R};\mathbb{C}) \times L^2(\mathbb{R};\mathbb{C}) \to \mathbb{C}, \quad \langle f,g \rangle := \int_{\mathbb{R}} f(x)\overline{g(x)} \, \mathrm{d}x.$$

And indeed, (5) allows such an expression. We just have to define the *linear operator*

$$Q : D(Q) \to L^2(\mathbb{R},\mathbb{C}) \text{ via } (Q\psi)(x) := x\psi(x), \text{ where } D(Q) := \left\{ \psi \in L^2(\mathbb{R};\mathbb{C}) : \int_{\mathbb{R}} x^2|\psi(x)|^2 \, \mathrm{d}x < \infty \right\}.$$

If we do so (5) can be rewritten as

$$\mu_\psi = \int_{\mathbb{R}} (Q\psi)(x)\overline{\psi(x)} \, \mathrm{d}x = \langle Q\psi, \psi \rangle.$$

We will often see expressions of the form $\langle T\psi,\psi \rangle$ appearing in our formulation (where T is a linear operator that is defined on a subset of $L^2(\mathbb{R};\mathbb{C})$. The operator Q is called *position operator.*

Definition 2.0.1 — Position operator

Let $D(Q) := \{\psi \in L^2(\mathbb{R};\mathbb{C}) : \int_{\mathbb{R}} x^2|\psi(x)|^2 \, \mathrm{d}x < \infty\}$. Then the *position operator* is given by

$$Q : D(Q) \to L^2(\mathbb{R};\mathbb{C}), \psi \mapsto Q\psi$$

where $Q\psi \in L^2(\mathbb{R};\mathbb{C})$ is the function that satisfies $(Q\psi)(x) = x\psi(x)$ for almost every $x \in \mathbb{R}$.

The position operator is the first example of a so-called *observable* — a concept which we are going to define now in full generality

Definition 2.0.2 — Observable and Expectation

Let $D(T)$ be a linear subspace of $L^2(\mathbb{R};\mathbb{C})$. A linear operator $T : D(T) \to L^2(\mathbb{R};\mathbb{C})$ is called *observable* with *domain* $D(T)$. For an observable T and a state function $\psi \in D(T)$ we define the *expectation* $\mu_\psi(T) := \langle T\psi, \psi\rangle$.

Oftentimes we will also ask that our observables are *symmetric*, we will discuss this important concept later.
A question we study now instead is: Can we also express the variance (given in (4)) in terms of Q? Yes, we can! To this end we however have to take the square of the operator Q, that is we define $D(Q^2) := \{\psi \in L^2(\mathbb{R};\mathbb{C}) : \psi \in D(Q), Q\psi \in D(Q)\}$ and form $Q^2 : D(Q^2) \to L^2(\mathbb{R};\mathbb{C}), Q^2\psi := Q(Q\psi)$. At first sight this seems more or less like a complicated way of writing up $Q \circ Q$, but one has to be careful with the domains of definition. Indeed, you can convince yourself that $x \mapsto \frac{1}{1+x^2}$ lies in $D(Q)$ but not in $D(Q^2)$. Anyways, for each $\psi \in D(Q^2)$ and almost every $x \in \mathbb{R}$ we have

$$(Q^2\psi)(x) = Q(Q\psi)(x) = x(Q\psi)(x) = x(x\psi(x)) = x^2\psi(x).$$

Now we write (with $I : L^2(\mathbb{R};\mathbb{C}) \to L^2(\mathbb{R};\mathbb{C})$ being shorthand for the identity)

$$\begin{aligned}
\mathrm{var}_\psi &= \int_{\mathbb{R}} (x-\mu_\psi)^2|\psi(x)|^2 \, \mathrm{d}x = \int_{\mathbb{R}} [x^2 - 2\mu_\psi x + \mu_\psi^2]\psi(x)\overline{\psi(x)} \, \mathrm{d}x \\
&= \int_{\mathbb{R}} [(Q^2\psi)(x) - 2\mu_\psi(Q\psi)(x) + \mu_\psi^2\psi(x)]\overline{\psi(x)} \, \mathrm{d}x \\
&= \langle (Q^2 - 2\mu_\psi Q + \mu_\psi^2 I)\psi, \psi\rangle = \langle (Q-\mu_\psi I)^2\psi, \psi\rangle,
\end{aligned}$$

where we formally have to define for $\mu \in \mathbb{R}$ the operator $(Q-\mu I)^2 : D(Q^2) \to L^2(\mathbb{R};\mathbb{C})$ via $(Q-\mu I)^2\psi := Q^2\psi - 2\mu Q\psi + \mu^2\psi$. Notice that the domain of definition of $(Q-\mu I)^2$ coincides with the domain of definition of Q^2 and all the quantities we formed in the definition are well defined. This will be of use later.
The position operator has a very special structure. In the future we will also study other more general observables (like e.g. the momentum operator). This is why we would like to define the variance in full generality.

Definition 2.0.3 — VARIANCE AND STANDARD DEVIATION

Let $T : D(T) \to L^2(\mathbb{R};\mathbb{C})$ be an observable. Define $D(T^2) := \{\psi \in L^2(\mathbb{R};\mathbb{C}), \psi \in D(T), T\psi \in D(T)\}$. For $\psi \in D(T^2)$ define the *variance*

$$\mathrm{var}_\psi(T) := \langle (T - \mu_\psi(T)I)^2\psi, \psi\rangle,$$

where for $\mu \in \mathbb{R}$ the linear operator $(T - \mu I)^2 : D(T^2) \to L^2(\mathbb{R};\mathbb{C})$ is given by $(T-\mu I)^2\psi := T^2\psi - 2\mu T\psi + \mu^2\psi$.

We also define the *standard deviation* $\mathrm{sd}_\psi(T) := \sqrt{\mathrm{var}_\psi(T)}$

2.1 Further Observables and their properties

Before we start we briefly recall the notion of the Sobolev space $W^{1,2}(\mathbb{R};\mathbb{C})$.

Definition 2.1.1 — WEAK DERVIATIVE, SOBOLEV SPACE

Let $f \in L^1_{\mathrm{loc}}(\mathbb{R};\mathbb{C})$. We say that f has weak derviative $g \in L^1_{\mathrm{loc}}(\mathbb{R};\mathbb{C})$ if

$$\int_{\mathbb{R}} f(x)\eta'(x)\,\mathrm{d}x = -\int_{\mathbb{R}} g(x)\eta(x)\,\mathrm{d}x \qquad \forall \eta \in C_0^\infty(\mathbb{R};\mathbb{C})$$

We define the Sobolev space $W^{1,2}(\mathbb{R};\mathbb{C})$ via

$$W^{1,2}(\mathbb{R};\mathbb{C}) := \{f \in L^2(\mathbb{R};\mathbb{C}) : f \text{ has a weak derivative that lies in } L^2(\mathbb{R};\mathbb{C})\}$$

For open intervals $I \subset \mathbb{R}$ one can also definie weak derivatives analogously . More precisely, we say that $f \in L^1_{\mathrm{loc}}(I;\mathbb{C})$ has weak derviative $g \in L^1_{\mathrm{loc}}(I;\mathbb{C})$ if

$$\int_{\mathbb{R}} f(x)\eta'(x)\,\mathrm{d}x = -\int_{\mathbb{R}} g(x)\eta(x)\,\mathrm{d}x \qquad \forall \eta \in C_0^\infty(I;\mathbb{C})$$

Analogously one can then define $W^{1,2}(I;\mathbb{C})$. Our analysis will only focus on the case $I = \mathbb{R}$, which is somewhat typical for Quantum mechanics. We will also see in this chapter why.

Remark 2.1.2

If $f \in L^1_{\mathrm{loc}}(\mathbb{R};\mathbb{C})$ is a weakly differentiable function on $\mathbb{R}$ then its weak derivative is uniquely determined by f (as an element of $L^1_{\mathrm{loc}}(\mathbb{R};\mathbb{C})$, i.e. only defined for Lebesgue-almost every x). Hence we may give it a name: The weak derivative of such f will from now on be called f'.

As discussed in the introduction a state function ψ is related to the probability distribution of the position of a particle on the real line. This is generalizing the concept of *position* to the quantum setting. Now we would like to generalize the concept of *velocity* (or, the comcept of momentum which is the product of mass and velocity). Velocity is the rate of change of the position, classically expressed by the derivative. This motivates the definition of the *momentum operator* as follows

Definition 2.1.3 — Momentum operator

We set $D(P) := W^{1,2}(\mathbb{R};\mathbb{C})$ and define the momentum operator $P : D(P) \to L^2(\mathbb{R};\mathbb{C})$ via

$$(P\psi)(x) := \frac{h}{2\pi i}\psi'(x),$$

for almost every $x \in \mathbb{R}$, where $\psi' \in L^2(\mathbb{R};\mathbb{C})$ denotes the weak Sobolev derivative.

We can also form expectations for the momentum operator. According to Definition 2.0.2 we have for $\psi \in D(P)$

$$\mu_\psi(P) := \langle P\psi, \psi\rangle = \frac{h}{2\pi i}\int_{\mathbb{R}} \psi'(x)\overline{\psi(x)}\,\mathrm{d}x.$$

2.1.1 Symmetric observables

Let $T : D(T) \to L^2(\mathbb{R};\mathbb{C})$ be an observable. In this section we study an important property that the observable T can have, which is *symmetry*.

Definition 2.1.4 — Symmetry

An observable $T : D(T) \to L^2(\mathbb{R};\mathbb{C})$ is called *symmetric* if for all $f, g \in D(T)$ we have

$$\langle Tf, g\rangle = \langle f, Tg\rangle$$

Let us compare this notion to its finite-dimensional analogue. If we have a linear operator $A : \mathbb{C}^n \to \mathbb{C}^n$ given we realize that the equation

$$\langle Ax, y\rangle = \langle x, Ay\rangle \qquad \text{for all } x, y \in \mathbb{C}^d$$

is equivalent to Hermitean(!) symmetry of the matrix M that represents A (that is, if $M \in \mathbb{C}^{n\times n}$ is such that $Ax = M \cdot x$ for all $x \in \mathbb{C}^n$ we have that $M = \overline{M}^T$). One should not forget the complex conjugate in this formula. It will play a role later that position and momentum operator are both symmetric.

Proposition 2.1.5

Let Q be as in Definition 2.0.1 and P be as in Definition 2.1.3. Then both Q and P are symmetric.

Proof (Part I). For Q this is easy to show. Suppose that $f, g \in D(Q)$. In particular f, g and $x \mapsto xf(x)$ and $x \mapsto xg(x)$ are functions in $L^2(\mathbb{R};\mathbb{C})$. Given this we may compute

$$\langle Qf, g\rangle = \int_{\mathbb{R}} (Qf)(x)\overline{g(x)}\,\mathrm{d}x = \int_{\mathbb{R}} xf(x)\overline{g(x)}\,\mathrm{d}x$$

$$\underset{x \in \mathbb{R}}{=\!=} \int_{\mathbb{R}} \overline{x} f(x)\overline{g(x)} \, \mathrm{d}x = \int_{\mathbb{R}} f(x)\overline{x g(x)} \, \mathrm{d}x = \langle f, Qg \rangle.$$

Symmetry of Q is shown. For symmetry of P we refer to the end of this section.

To prove the symmetry of P we need a preparatory lemma.

Lemma 2.1.6 — Sobolev Approximation on the real line

Suppose that $f \in W^{1,2}(\mathbb{R};\mathbb{C})$ has weak derivative f'. Then there exists a sequence $(\eta_n)_{n\in\mathbb{N}} \subset C_0^\infty(\mathbb{R};\mathbb{C})$ such that $\eta_n \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f$ and $\eta_n' \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f'$

Proof. Let $f \in W^{1,2}(\mathbb{R};\mathbb{C})$ be as in the statement. Let $\theta \in C_0^\infty(\mathbb{R})$ be such that $\theta|_{B_1(0)} \equiv 1$ and $\theta|_{\mathbb{R}\setminus B_2(0)} \equiv 0$. Define first for $n \in \mathbb{N}$ the function $f_n : \mathbb{R} \to \mathbb{R}$ via $f_n(x) := f(x)\theta(\frac{x}{n})$.

Intermediate Claim 1. For all $n \in \mathbb{N}$ we have $f_n \in W^{1,2}(\mathbb{R};\mathbb{C})$, $f_n \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f$ and $f_n' \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f'$.

Let $n \in \mathbb{N}$. We first show that f_n is weakly differentiable. To this end let $\varphi \in C_0^\infty(\mathbb{R};\mathbb{C})$ be arbitrary. We compute

$$\begin{aligned}\int_{\mathbb{R}} f_n(x)\varphi'(x) \, \mathrm{d}x &= \int_{\mathbb{R}} f(x)\theta(\tfrac{x}{n})\varphi'(x) \, \mathrm{d}x \\ &= \int_{\mathbb{R}} f(x)\frac{d}{dx}(\theta(\tfrac{x}{n})\varphi(x)) \, \mathrm{d}x - \int_{\mathbb{R}} f(x)\tfrac{1}{n}\theta'(\tfrac{x}{n})\varphi(x) \, \mathrm{d}x.\end{aligned}$$

Here we have used the product rule of differentiation in the last step (read it backwards!). Noticing that $x \mapsto \theta(\frac{x}{n})\varphi(x)$ lies in $C_0^\infty(\mathbb{R};\mathbb{C})$ we may use the definition of the weak derivative in the first integral to obtain

$$\begin{aligned}\int_{\mathbb{R}} f_n(x)\varphi'(x) \, \mathrm{d}x &= -\int_{\mathbb{R}} f'(x)\theta(\tfrac{x}{n})\varphi(x) \, \mathrm{d}x - \int_{\mathbb{R}} f(x)\tfrac{1}{n}\theta'(\tfrac{x}{n})\varphi(x) \, \mathrm{d}x \\ &= -\int_{\mathbb{R}} (f'(x)\theta(\tfrac{x}{n}) + \tfrac{1}{n}f(x)\theta'(\tfrac{x}{n}))\varphi(x) \, \mathrm{d}x.\end{aligned}$$

Since φ was arbitrary we infer that f_n is weakly differentiable with weak derivative

$$f_n'(x) = f'(x)\theta(\tfrac{x}{n}) + \tfrac{1}{n}f(x)\theta'(\tfrac{x}{n}) \quad (\text{a.e. } x \in \mathbb{R}),$$

which is intuitive due to the product rule. We leave as an exercise to show that f_n, f_n' are square integrable. It remains to show that $f_n \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f$ and $f_n' \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f'$. For the first claim we look at

$$\|f_n - f\|_{L^2}^2 = \int_{\mathbb{R}} |f(x)\theta(\tfrac{x}{n}) - f(x)|^2 \, \mathrm{d}q = \int_{\mathbb{R}} |f(x)|^2 |1-\theta(\tfrac{x}{n})|^2 \, \mathrm{d}q.$$

Now observe that $|1-\theta(\frac{x}{n})|^2 \xrightarrow{n\to\infty} 0$ for each $x \in \mathbb{R}(^a)$ and $|f(x)|^2|1-\theta(\frac{x}{n})|^2 \leqslant (1+\sup_{\mathbb{R}}\theta)^2|\,|f(x)|^2$, which lies in $L^1(\mathbb{R})$ (due to the fact that θ is bounded on $\mathbb{R}$). Hence the dominated convergence theorem applies and yields $\lim\limits_{n\to\infty}\|f_n - f\|_{L^2}^2 = 0$. For the convergence of the derivatives we compute

$$\begin{aligned}\|f_n' - f'\|_{L^2}^2 &= \int_{\mathbb{R}} |f'(x)\theta(\tfrac{x}{n}) + \tfrac{1}{n}f(x)\theta'(\tfrac{x}{n}) - f'(x)|^2 \, \mathrm{d}x \\ &= \int_{\mathbb{R}} |f'(x)(\theta(\tfrac{x}{n}) - 1) + \tfrac{1}{n}f(x)\theta'(\tfrac{x}{n})|^2 \, \mathrm{d}x \\ &\leqslant 2\int_{\mathbb{R}} |f'(x)|^2|\theta(\tfrac{x}{n}) - 1|^2 + \tfrac{2}{n^2}\int_{\mathbb{R}} |f(x)|^2|\theta'(\tfrac{x}{n})|^2 \, \mathrm{d}x,\end{aligned}$$

where we have used the standard inequality $|a+b|^2 \leqslant 2(|a|^2+|b|^2)$ in the last step. That the first integrand goes to zero can be shown with a very similar technique as above. The second integrand can be discussed as follows. We may estimate $|\theta'(\frac{q}{n})|^2 \leqslant \sup_{\mathbb{R}}|\theta'|^2 := C$ (which is finite due to the fact that $|\theta'|^2$ is a continuous function with compact support) and obtain that the second integral is bounded above by $\frac{2C}{n^2}\|f\|_{L^2}^2 \xrightarrow{n\to\infty} 0$. This yields that also the second integral tends to zero and we infer $\lim\limits_{n\to\infty}\|f_n' - f'\| = 0$. The intermediate claim is shown.

Intermediate Claim 2. Suppose that $g \in W^{1,2}(\mathbb{R};\mathbb{C})$ is such that there exists some compact set $K \subset \mathbb{R}$ with $g|_{\mathbb{R}\setminus K} = 0$ (a.e.). Then for each $\varepsilon > 0$ there exists $g_\varepsilon \in C_0^\infty(\mathbb{R};\mathbb{C})$ such that $\|g - g_\varepsilon\|_{L^2} + \|g' - g_\varepsilon'\|_{L^2} < \varepsilon$.

The proof of this fact is left to the reader as an exercise and takes advantage of approximations to the identity (as seen in Santiago's Part).

Now we turn to the actual proof. Let $f \in W^{1,2}(\mathbb{R};\mathbb{C})$ and $(f_n)_{n\in\mathbb{N}}$ be as in Intermediate Claim 1. One readily checks that $f_n|_{\mathbb{R}\setminus\overline{B_{3n}(0)}} = 0$. In particular, we may apply Intermediate Claim 2 with $g = f_n$, $K = \overline{B_{3n}(0)}$ and $\varepsilon = \frac{1}{n}$. As a result we obtain some $\eta_n \in C_0^\infty(\mathbb{R};\mathbb{C})$ such that $\|f_n - \eta_n\|_{L^2} + \|f_n' - \eta_n'\|_{L^2} < \frac{1}{n}$. The triangle inequality in L^2 yields

$$\|f - \eta_n\|_{L^2} \leqslant \|f - f_n\|_{L^2} + \|f_n - \eta_n\|_{L^2} \leqslant \|f - f_n\|_{L^2} + \tfrac{1}{n} \xrightarrow{n\to\infty} 0$$

and

$$\|f' - \eta_n'\|_{L^2} \leqslant \|f' - f_n'\|_{L^2} + \|f_n' - \eta_n'\|_{L^2} \leqslant \|f' - f_n'\|_{L^2} + \tfrac{1}{n} \xrightarrow{n\to\infty} 0.$$

The claim follows.

[a] Indeed: For $x \in \mathbb{R}$ and $n > |x|$ we have $\eta(\frac{x}{n}) = 1$ and thus $|1 - \theta(\frac{x}{n})|^2 = 0$ for all $n > |x|$.

Remark 2.1.7

Lemma 2.1.6 is highly nontrivial: If one replaces the domain of definition $\mathbb{R}$ by some bounded interval $(0,1)$ the conclusion fails to hold, even for $f \equiv 1$ (which lies in $W^{1,2}((0,1);\mathbb{C})$ and has weak derivative 0). More precisely

There exists no sequence $(\eta_n)_{n\in\mathbb{N}} \subset C_0^\infty((0,1);\mathbb{C})$ such that $\eta_n \xrightarrow[L^2]{n\to\infty} 1$ and $\eta_n' \xrightarrow[L^2]{n\to\infty} 0$.

To see this assume the opposite, i.e. assume that $(\eta_n)_{n\in\mathbb{N}} \subset C_0^\infty((0,1);\mathbb{C})$ is such that $\eta_n \xrightarrow[L^2]{n\to\infty} 1$ and $\eta_n' \xrightarrow[L^2]{n\to\infty} 0$. By extending η_n by zero on $\mathbb{R}\backslash(0,1)$ we may regard $(\eta_n)_{n\in\mathbb{N}}$ as a sequence in $C_0^\infty(\mathbb{R};\mathbb{C})$ that satisfies $\operatorname{spt}(\eta_n) \subseteq (0,1)$ for all $n \in \mathbb{N}$. The fundamental theorem of calculus yields that for $n \in \mathbb{N}$ and $x \in (0,1)$ we have

$$\begin{aligned}|\eta_n(x)| &= \left|\eta_n(0) + \int_0^x \eta_n'(s)\,\mathrm{d}s\right| = \left|\int_0^x \eta_n'(s)\,\mathrm{d}s\right| \leqslant \int_0^x |\eta_n'(s)|\,\mathrm{d}s \\ &\leqslant \int_0^1 |\eta_n'(s)|\,\mathrm{d}s \leqslant \sqrt{\int_0^1 |\eta_n'(s)|^2\,\mathrm{d}s}\sqrt{\int_0^1 1\,\mathrm{d}s} = \|\eta_n'\|_{L^2}.\end{aligned}$$

As a result we obtain

$$\|\eta_n\|_{L^2}^2 = \int_0^1 |\eta_n(x)|^2\,\mathrm{d}x \leqslant \int_0^1 \|\eta_n'\|_{L^2}^2\,\mathrm{d}x = \|\eta_n'\|_{L^2}^2 \xrightarrow{n\to\infty} 0.$$

But then (by the inverse triangle inequality)

$$\|\eta_n - 1\|_{L^2} \geqslant \big|\,\|1\|_{L^2} - \|\eta_n\|_{L^2}\,\big| \xrightarrow{n\to\infty} |1-0| = 1,$$

which contradicts $\eta_n \xrightarrow[L^2]{n\to\infty} 1$ in L^2.

Proof (of Proposition 2.1.5, **Part II**). We must now show the symmetry of P. To this end suppose that $f, g \in D(P) = W^{1,2}(\mathbb{R};\mathbb{C})$. Before we start we leave it as an exercise to show that $\overline{g} \in W^{1,2}(\mathbb{R};\mathbb{C})$ with $\overline{g}' = \overline{g'}$ (!). By Lemma 2.1.6 we can find $(\eta_n)_{n\in\mathbb{N}} \subset C_0^\infty(\mathbb{R};\mathbb{C})$ such that $\eta_n \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f$ and $\eta_n' \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} f'$. As a result we may compute

$$\begin{aligned}\langle Pf, g\rangle &= \frac{h}{2\pi i}\int_{\mathbb{R}} f'(x)\overline{g(x)}\,\mathrm{d}x = \lim_{n\to\infty}\frac{h}{2\pi i}\int_{\mathbb{R}} \eta_n'(x)\overline{g(x)}\,\mathrm{d}x \\ &\underset{(!)}{=} \lim_{n\to\infty}\frac{-h}{2\pi i}\int_{\mathbb{R}} \eta_n(x)\overline{g'(x)}\,\mathrm{d}x = \frac{-h}{2\pi i}\int_{\mathbb{R}} f(x)\overline{g'(x)}\,\mathrm{d}x\end{aligned}$$

$$= \overline{\frac{h}{2\pi i}} \int_{\mathbb{R}} f(x)\overline{g'(x)}\, \mathrm{d}x = \int_{\mathbb{R}} f(x)\overline{\frac{h}{2\pi i} g'(x)}\, \mathrm{d}x = \langle f, Pg\rangle.$$

The claimed symmetry follows.

Remark 2.1.8

We would like to conclude this section with a remark why symmetry of is a meaningful assumption of observables in physics. The reason is the following

Observation. If $T : D(T) \to L^2(\mathbb{R}^d;\mathbb{C})$ is a symmetric observable then for each $\psi \in D(T)$ we have $\mu_\psi(T) = \langle T\psi, \psi\rangle \in \mathbb{R}$.

This is easily seen as follows. For $\psi \in D(T)$ we have due to symmetry of T and Hermitean symmetry of $\langle \cdot, \cdot\rangle$

$$\langle T\psi, \psi\rangle = \langle \psi, T\psi\rangle = \int_{\mathbb{R}} \psi(x)\overline{(T\psi)(x)}\, \mathrm{d}x = \overline{\int_{\mathbb{R}} \overline{\psi(x)} T\psi(x)\, \mathrm{d}x} = \overline{\langle T\psi, \psi\rangle}.$$

For this reason $\langle T\psi, \psi\rangle$ is a real number.

2.2 Commutators and Heisenberg's uncertainty principle

The position operator and the momentum operator do not *commute*. That means, roughly speaking, that it makes a difference which quantity we measure first: Position or Momentum. A very rough way to write this mathematically is $PQ \neq QP$. However one must be a bit careful when writing such a relation, since both operators P and Q have different domains of definition. To be precise what we mean here we define

Definition 2.2.1 — Composition of Observables

Let $T : D(T) \to L^2(\mathbb{R};\mathbb{C})$ and $S : D(S) \to L^2(\mathbb{R};\mathbb{C})$ be observables. We define $D(TS) := \{\psi \in D(S) : S\psi \in D(T)\}$ and

$$TS : D(TS) \to L^2(\mathbb{R};\mathbb{C}), \qquad (TS)\psi := T(S\psi).$$

As already mentioned it does in general make a difference which operator is applied first, T or S (even in the domain of definition). To describe precisely what difference it makes we discuss the *commutator*.

Definition 2.2.2 — Commutator

Let $T : D(T) \to L^2(\mathbb{R};\mathbb{C})$ and $S : D(S) \to L^2(\mathbb{R};\mathbb{C})$ be observables. Then we define

$D([S,T]) := D(ST) \cap D(TS)$ and call $[S,T] : D([S,T]) \to L^2(\mathbb{R},\mathbb{C}), [S,T]\psi = (ST)\psi - (TS)\psi$ the *commutator* of S and T.

As an example we compute a formula for the commutator of $P$and Q, which is commonly referred to as *Heisenberg's commutation relation*

Proposition 2.2.3 — HEISENBERG'S COMMUTATION RELATION

Suppose that $\psi \in D([P,Q])$. Then

$$[P,Q]\psi = \frac{h}{2\pi i}\psi.$$

Proof. We compute (for a.e. $x \in \mathbb{R}$)

$$(PQ\psi)(x) = P(Q\psi)(x) = \frac{h}{2\pi i}(Q\psi)'(x).$$

Using that $(Q\psi)(x) = x\psi(x)$ for all $x \in \mathbb{R}$ we can readily check that $(Q\psi)'$ is given by $(Q\psi)'(x) = \psi(x) + x\psi'(x)$. (This is not surprising in view of the product rule but one has to verify this also in terms of weak derivatives). Given this formula we obtain for a.e. $x \in \mathbb{R}$

$$(PQ\psi)(x) = \frac{h}{2\pi i}\psi(x) + \frac{h}{2\pi i}x\psi'(x).$$

Moreover, one readily checks that $(QP\psi)(x) = \frac{h}{2\pi i}x\psi'(x)$. This yields

$$([P,Q]\psi)(x) = \frac{h}{2\pi i}\psi(x) + \frac{h}{2\pi i}x\psi'(x) - \frac{h}{2\pi i}x\psi'(x) = \frac{h}{2\pi i}\psi(x) \quad \text{for a.e } x \in \mathbb{R}.$$

The claim follows.

The next theorem, called *commutator theorem* relates the expectation of the commutator and the variances of the operators

Theorem 2.2.4 — COMMUTATOR THEOREM

Let $S : D(S) \to L^2(\mathbb{R};\mathbb{C}), T : D(T) \to L^2(\mathbb{R},\mathbb{C})$ be symmetric observables and $\psi \in D([S,T]) \cap D(T^2) \cap D(S^2)$. Then

$$|\mu_\psi([S,T])|^2 \leqslant 4\mathrm{var}_\psi(S)\mathrm{var}_\psi(T).$$

Proof. Recall first that $\psi \in D([S,T]) = D(ST) \cap D(TS)$ means $\psi \in D(T)$ and $T\psi \in D(S)$ as well as $\psi \in D(S)$ and $S\psi \in D(T)$. Define $\mu_1 := \mu_\psi(S)$ and $\mu_2 := \mu_\psi(T)$ as well as the observables $A := S - \mu_1 I$ (defined on $D(S)$) and $B := T - \mu_2 I$ (defined on $D(T)$). One readily checks that $D([A,B]) = D([S,T])$ and

$$[A,B] = AB - BA = (S - \mu_1 I)(T - \mu_2 I) - (T - \mu_2 I)(S - \mu_1 I)$$

$$= ST - \mu_1 T - \mu_2 S + \mu_1\mu_2 I - (TS - \mu_1 T - \mu_2 S + \mu_1\mu_2 I) = ST - TS = [S,T].$$

For this reason we have

$$\mu_\psi([S,T]) = \mu_\psi([A,B]) = \langle AB\psi - BA\psi, \psi\rangle = \langle AB\psi, \psi\rangle - \langle BA\psi, \psi\rangle. \tag{6}$$

Since A is now symmetric and $B\psi, \psi \in D(A)$ we have $\langle AB\psi, \psi\rangle = \langle B\psi, A\psi\rangle$. Moreover, given that $A\psi, \psi \in D(B)$ we have (by symmetry of B) $\langle BA\psi, \psi\rangle = \langle A\psi, B\psi\rangle$, so that (6) yields

$$\mu_\psi([S,T]) = \langle B\psi, A\psi\rangle - \langle A\psi, B\psi\rangle.$$

Taking absolute values and using the triangle (can Cauchy-Schwarz inequality we obtain

$$|\mu_\psi([S,T])| = |\langle B\psi, A\psi\rangle - \langle A\psi, B\psi\rangle| \leqslant |\langle B\psi, A\psi\rangle| + |\langle A\psi, B\psi\rangle| \leqslant 2\|B\psi\|_{L^2}\|A\psi\|_{L^2},$$

i.e.

$$|\mu_\psi([S,T])|^2 \leqslant 4\|B\psi\|_{L^2}^2\|A\psi\|_{L^2}^2 \tag{7}$$

Now note that due to the fact that $\psi, B\psi \in D(B)$ we have

$$\|B\psi\|_{L^2}^2 = \langle B\psi, B\psi\rangle = \langle B(B\psi), \psi\rangle = \langle B^2\psi, \psi\rangle = \langle (T - \mu_2 I)^2\psi, \psi\rangle = \mathrm{var}_\psi(T).$$

Similarly we find $\|A\psi\|_{L^2}^2 = \mathrm{var}_\psi(S)$ and the claim follows from (7).

A direct consequence is *Heisenberg's uncertainty principle*

Theorem 2.2.5 — HEISENBERG'S UNCERTAINTY PRINCIPLE

Suppose that $\psi \in D([P,Q]) \cap D(P^2) \cap D(Q^2)$ is such that $\int_{\mathbb{R}} |\psi(x)|^2 \,\mathrm{d}x = 1$. Then

$$\mathrm{var}_\psi(P)\mathrm{var}_\psi(Q) \geqslant \frac{h^2}{16\pi^2}.$$

Proof. Let ψ be as in the statement. Then (2.2.3) yields $[P,Q]\psi = \frac{h}{2\pi i}\psi$. As a result we have

$$\mu_\psi([P,Q]) = \langle [P,Q]\psi, \psi\rangle = \frac{h}{2\pi i}\int_{\mathbb{R}} \psi(x)\overline{\psi(x)} \,\mathrm{d}x = \frac{h}{2\pi i}\int_{\mathbb{R}} |\psi(x)|^2 \,\mathrm{d}x = \frac{h}{2\pi i}.$$

Using this and Theorem 2.2.4 (applicable since P and Q are symmetric, cf. Proposition 2.1.5) we find

$$\frac{h^2}{4\pi^2} \leqslant |\mu_\psi([P,Q])|^2 \leqslant 4\mathrm{var}_\psi(P)\mathrm{var}_\psi(Q),$$

so that

$$\mathrm{var}_\psi(P)\mathrm{var}_\psi(Q) \geqslant \frac{h^2}{16\pi^2}.$$

This shows in particular one thing: No matter how the probability distribution looks like: P and Q can not both be deterministic: If the variance of the position operator Q is small then we have $\mathrm{var}_\psi(P) \geqslant \frac{h^2}{16\pi^2 \mathrm{var}_\psi(Q)}$ so that the variance of the momentum operator is big.

09.06.2026

2.2.1 Quantum mechanics and Fourier transform

In the following we will assume for simplicity that $h = 2\pi$. In particular, the momentum operator is given by $(P\psi)(x) = \frac{1}{i}\psi'(x)$ for a.e. $x \in \mathbb{R}$ (for any $\psi \in W^{1,2}(\mathbb{R};\mathbb{C})$).

2.2.1.1 Preliminaries about the Fourier transform In this part of the lecture we define the Fourier transform on $\mathbb{R}$ as follows:

Definition 2.2.6 — Fourier Transform

Let $f \in \mathcal{S}(\mathbb{R};\mathbb{C})$. We define the *Fourier Transform* $\mathcal{F}(f) : \mathbb{R} \to \mathbb{C}$ of f to be

$$\mathcal{F}(f)(p) := \hat{f}(p) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x) e^{-ip\cdot x}\, \mathrm{d}x.$$

Moreover we define the *Inverse Fourier Transform* $\mathcal{F}^{-1}(f) : \mathbb{R} \to \mathbb{C}$ via

$$\mathcal{F}^{-1}(f)(x) := \check{f}(x) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(p) e^{ip\cdot x}\, \mathrm{d}p.$$

Note that the prefactor $\frac{1}{\sqrt{2\pi}}$ differs slightly from the prefactor that was used in Part II of the lecture. This new convention will however be more suitable for our purposes which is why we redefine the Fourier Transform now.

Remark 2.2.7 — Properties of the Fourier Transform

We will use several properties of the Fourier Transform, which we list here

- For all $f \in \mathcal{S}(\mathbb{R};\mathbb{C})$ we have $\mathcal{F}(f), \mathcal{F}^{-1}(f) \in \mathcal{S}(\mathbb{R};\mathbb{C})$
- $\mathcal{F}^{-1}(\mathcal{F}(f)) = \mathcal{F}(\mathcal{F}^{-1}(f)) = f$ for all $f \in \mathcal{S}(\mathbb{R};\mathbb{C})$
- For all $f \in \mathcal{S}(\mathbb{R};\mathbb{C})$ we have $\mathcal{F}(f)' = -i\mathcal{F}(x \mapsto xf(x))$
- For all $f \in \mathcal{S}(\mathbb{R};\mathbb{C})$ and $p \in \mathbb{R}$ we have $\mathcal{F}(f')(p) = ip\mathcal{F}(f)(p)$
- For all $f \in \mathcal{S}(\mathbb{R};\mathbb{C})$ we have

$$\int_{\mathbb{R}} |f(x)|^2\, \mathrm{d}x = \int_{\mathbb{R}} |\mathcal{F}(f)(p)|^2\, \mathrm{d}p.$$

For proofs of all these properties we refer to Part II of the lecture.

Remark 2.2.8

Note also that the Fourier transform generalizes in a straightforward way to functions in $\mathcal{S}(\mathbb{R}^d;\mathbb{C})$ when defining for $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ the Fourier transform $\mathcal{F}(f) : \mathbb{R}^d \to \mathbb{C}$ via

$$\mathcal{F}(f)(p) := \hat{f}(p) := \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} f(x) e^{-ip\cdot x} \, \mathrm{d}x \tag{8}$$

with "$\cdot$" denoting the canonical scalar product on $\mathbb{R}^d$. The formula for the inverse Fourier transform $\mathcal{F}^{-1}(f) : \mathbb{R}^d \to \mathbb{C}$ is also very canonical

$$\mathcal{F}^{-1}(f)(x) := \check{f}(p) := \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} f(p) e^{ip\cdot x} \, \mathrm{d}p.$$

The properties from the previous remark carry over in a straighforward way, i.e.

- For all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we have $\mathcal{F}(f), \mathcal{F}^{-1}(f) \in \mathcal{S}(\mathbb{R}d;\mathbb{C})$
- $\mathcal{F}^{-1}(\mathcal{F}(f)) = \mathcal{F}(\mathcal{F}^{-1}(f)) = f$ for all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$
- For all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we have $\partial_i \mathcal{F}(f) = i\mathcal{F}(x \mapsto x_i f)$
- For all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ and $p \in \mathbb{R}^d$ we have $\mathcal{F}(\partial_i f)(p) = -ip_i \mathcal{F}(f)(p)$
- For all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we have

$$\int_{\mathbb{R}^d} |f(x)|^2 \, \mathrm{d}x = \int_{\mathbb{R}^d} |\mathcal{F}(f)(p)|^2 \, \mathrm{d}p.$$

The Fourier Transform extends canonically to a linear map $\mathcal{F} : \mathcal{S}'(\mathbb{R}^d;\mathbb{C}) \to \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$.

Definition 2.2.9 — Fourier Transform on $\mathcal{S}'(\mathbb{R}^d;\mathbb{C})$

Let $L : \mathcal{S}(\mathbb{R}^d;\mathbb{C}) \to \mathbb{C}$ be a tempered distribution, i.e. $L \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ be a tempered distribution. Then we define $\mathcal{F}(L) \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ via the formula

$$\mathcal{F}(L)(\varphi) := L(\hat{\varphi}) \qquad \text{for all } \varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$$

What is maybe less known is that we may also look at $\mathcal{F}$ as a bijective operator on $L^2(\mathbb{R}^d;\mathbb{C})$. This has been discussed in Theorem 6.14 of Part II, but I would like to provide a bit more details. While the above definition and the fact that $L^2(\mathbb{R}^d;\mathbb{C}) \subseteq \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ allows us already to apply $\mathcal{F}$ on any L^2-function it is not clear that the image maps bijectively onto $L^2(\mathbb{R}^d;\mathbb{C})$. If we write $L^2(\mathbb{R}^d;\mathbb{C}) \subseteq \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ we of course have to specify what we mean by that (since we need to identify functions with distributions). We precisely mean that to $g \in L^2(\mathbb{R}^d;\mathbb{C})$ we associate the tempered distribution

$$L_g : \mathcal{S}(\mathbb{R}^d;\mathbb{C}) \to \mathbb{C}, \qquad L_g(\varphi) := \int_{\mathbb{R}^d} g\varphi \, \mathrm{d}x \tag{9}$$

which lies (as one readily checks) in $\mathcal{S}'(\mathbb{R}^d;\mathbb{C})$.

Theorem 2.2.10 — Fourier Transform on $L^2(\mathbb{R}^d;\mathbb{C})$

There exists a unique bijective linear map $\mathcal{F} : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ such that $\mathcal{F}(f) = \hat{f}$ for all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Moreover, $\mathcal{F}$ is unitary, i.e. for all $f \in L^2(\mathbb{R}^d;\mathbb{C})$ there holds $\|\mathcal{F}(f)\|_{L^2} = \|f\|_{L^2}$. Furthermore, $\mathcal{F}$ coincides with the distributional Fourier transform in Definition 2.2.9 in the following sense: With the notation of (9) we have $L_{\mathcal{F}(f)} = \mathcal{F}(L_f)$ (with $\mathcal{F}(L_f)$ being as in Definition 2.2.9)

Proof. (!Functional Analysis!)

Step 1. Construction

We first will define the map $\mathcal{F}$. This is not straightforward as for general $f \in L^2(\mathbb{R}^d;\mathbb{C})$ the integral in (8) is not necessarily convergent. To this end let $f \in L^2(\mathbb{R}^d;\mathbb{C})$. It is known that then there exists $(\eta_n)_{n\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ such that $\eta_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} f$. (Indeed one can even take $(\eta_n)_{n\in\mathbb{N}} \subseteq C_0^\infty(\mathbb{R}^d;\mathbb{C})$). In particular $(\eta_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2(\mathbb{R}^d;\mathbb{C})$. Observe that $\mathcal{F}(\eta_n) = \hat{\eta}_n$ can already be computed by means of (8), we just need to find a way to compute $\mathcal{F}(f)$. To this end notice that for $m, n \in \mathbb{N}$ we have (given that the Fourier transform preserves the L^2-norm of Schwartz functions by Remark 2.2.8)

$$\|\mathcal{F}(\eta_m) - \mathcal{F}(\eta_n)\|_{L^2} = \|\mathcal{F}(\eta_m - \eta_n)\|_{L^2} \underset{\text{Rem2.2.8}}{=\!=\!=} \|\eta_m - \eta_n\|_{L^2}$$

For this reason $(\mathcal{F}(\eta_n))_{n\in\mathbb{N}} \subset L^2(\mathbb{R}^d;\mathbb{C})$ is a Cauchy sequence. Since $L^2(\mathbb{R}^d;\mathbb{C})$ is complete, this sequence has a limit in $L^2(\mathbb{R}^d;\mathbb{C})$. We would now like to define

$$\mathcal{F}(f) := \underset{n\to\infty}{\mathrm{LIM}}\, \mathcal{F}(\eta_n) \qquad \text{where } \underset{n\to\infty}{\mathrm{LIM}} \text{ refers to the } L^2(\mathbb{R}^d;\mathbb{C})\text{-limit of functions} \tag{10}$$

but this is only well-defined if the limit on the right hand side is independent of the chosen approximating sequence $(\eta_n)_{n\in\mathbb{N}}$. We will show next that this is the case. If $(\eta_n)_{n\in\mathbb{N}}, (\tilde{\eta}_n)_{n\in\mathbb{N}} \subseteq \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ are such that $\eta_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} f, \tilde{\eta}_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} f$ then $\eta_n - \tilde{\eta}_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$ and therefore

$$\|\mathcal{F}(\eta_n) - \mathcal{F}(\tilde{\eta}_n)\|_{L^2} = \|\mathcal{F}(\eta_n - \tilde{\eta}_n)\|_{L^2} = \|\eta_n - \tilde{\eta}_n\|_{L^2} \xrightarrow{n\to\infty} 0.$$

This implies that

$$\underset{n\to\infty}{\mathrm{LIM}}\, \mathcal{F}(\eta_n) = \underset{n\to\infty}{\mathrm{LIM}}\, \mathcal{F}(\tilde{\eta}_n)$$

and thus (10) becomes well-defined. The construction also immediately implies that $\mathcal{F}(f) = \hat{f}$ for all $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Indeed, if $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ one may choose $(\eta_n)_{n\in\mathbb{N}} = (f)_{n\in\mathbb{N}}$ and observe that $\mathcal{F}(\eta_n) = \hat{f}$ for all n to conclude that

$$\mathcal{F}(f) = \underset{n\to\infty}{\mathrm{LIM}}\, \hat{f} = \hat{f}.$$

Step 2. Preservation of L^2-norm, Linearity and Bijectivity.

Let us first derive the preservation of the L^2-norm. This follows readily from the construction. Indeed, let $f \in L^2(\mathbb{R}^d;\mathbb{C})$. Then choose $(\eta_n)_{n\in\mathbb{N}} \subseteq \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ in such a way that $\eta_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} f$. Given that $\mathcal{F}(f) = \operatorname*{LIM}_{n\to\infty} \mathcal{F}(\eta_n)$ we conclude

$$\|\mathcal{F}(f)\|_{L^2} = \lim_{n\to\infty} \|\mathcal{F}(\eta_n)\|_{L^2} = \lim_{n\to\infty} \|\hat{\eta_n}\|_{L^2} \underset{\text{Rem2.2.8}}{=\!=\!=} \lim_{n\to\infty} \|\eta_n\|_{L^2} = \|f\|_{L^2}.$$

The claim follows. The linearity of $\mathcal{F}$ follows similarly from the fact that linearity of $\mathcal{F}|_{\mathcal{S}(\mathbb{R}^d;\mathbb{C})}$ is directly evident from (8). We leave this to the reader as an exercise. Bijectivity follows if we extend the inverse Fourier transform to $L^2(\mathbb{R}^d;\mathbb{C})$ in the same manner as in Step 1. Also these details are left to the reader as an exercise.

Step 3. Consistency with the distributional Fourier Transform.

Recall from Part II (Proof of Theorem 4.5 Step 2) that for all $\eta_1, \eta_2 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we have

$$\int_{\mathbb{R}^d} \hat{\eta}_1(x)\eta_2(x)\,\mathrm{d}x = \int_{\mathbb{R}^d} \eta_1(x)\hat{\eta}_2(x)\,\mathrm{d}x \tag{11}$$

Now let $(\eta_n)_{n\in\mathbb{N}}$ be such that $\eta_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} f$. Then by our construction $\hat{\eta}_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \mathcal{F}(f)$. As a result we find for each $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$

$$\begin{aligned} L_{\mathcal{F}(f)}(\varphi) &= \int_{\mathbb{R}^d} \mathcal{F}(f)\varphi\,\mathrm{d}x \\ &= \lim_{n\to\infty} \int_{\mathbb{R}^d} \hat{\eta}_n\varphi\,\mathrm{d}x \underset{(11)}{=} \lim_{n\to\infty} \int_{\mathbb{R}^d} \eta_n\hat{\varphi}\,\mathrm{d}x = \int_{\mathbb{R}^d} f\hat{\varphi}\,\mathrm{d}x = L_f(\hat{\varphi}) = \mathcal{F}(L_f)(\varphi). \end{aligned}$$

The claim follows.

2.2.1.2 Fourier Transform and Momentum Space

Fourier transforms have the property of transforming derivatives into multiplications and back. Now the position operator is a multiplication and the momentum operator is a derivative. In particular, after Fourier transform they play seemingly the same role. More precisely: Recall that

$$Q : D(Q) \to L^2(\mathbb{R};\mathbb{C}) \quad (Q\psi)(x) = x\psi(x),$$

Now $P : D(P) \to L^2(\mathbb{R};\mathbb{C})$ satisfies $(P\psi)(x) = \frac{1}{i}\psi'(x)$. If we apply the Fourier transform (for simplicity in the special case $\psi \in \mathcal{S}(\mathbb{R};\mathbb{C})$) we have (by Remark 2.2.7)

$$\widehat{(P\psi)}(p) = \tfrac{1}{i}\widehat{\psi'}(p) = \tfrac{1}{i}ip\hat{\psi}(p) = p\hat{\psi}(p) = (Q\hat{\psi})(p).$$

With other words we have $\mathcal{F}(P\psi) = Q\mathcal{F}(\psi)$. Shorthand we would write $P = \mathcal{F}^{-1}Q\mathcal{F}$ holds on $\mathcal{S}(\mathbb{R};\mathbb{C})$. We will next discuss that this formula holds actually on all of $D(P)$!

Proposition 2.2.11
Let $\psi \in D(P)$. Then $\mathcal{F}(\psi) \in D(Q)$ and

$$P\psi = \mathcal{F}^{-1}Q\mathcal{F}\psi$$

Proof. Recall that $D(P) = W^{1,2}(\mathbb{R};\mathbb{C})$.

Intermediate claim. $\mathcal{F}(\psi')(p) = ip\mathcal{F}(\psi)(p)$ for Lebesgue almost-every $p \in \mathbb{R}$.

This would be immediate if $\psi \in \mathcal{S}(\mathbb{R};\mathbb{C})$ (see Remark 2.2.7), but in our situation we have significantly less regularity (only $W^{1,2}$). This is why we proceed as follows. Lemma 2.1.6 allows us to choose $(\eta_n)_{n\in\mathbb{N}} \subset C_0^\infty(\mathbb{R};\mathbb{C})$ such that $\eta_n \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} \psi$ and $\eta_n' \xrightarrow[L^2(\mathbb{R};\mathbb{C})]{n\to\infty} \psi'$. Using that $\mathcal{F}$ is an isometry (and hence continuous) in L^2 we find that $\mathcal{F}(\eta_n) \xrightarrow{L^2} \mathcal{F}(\psi)$ and $\mathcal{F}(\eta_n') \xrightarrow{L^2} \mathcal{F}(\psi')$. Proposition 2.3.17 in ↑ `Analysis III Lecture Notes` yields that there exists a subsequence $(\ell_n)_{n\in\mathbb{N}} \subset \mathbb{N}$ such that $\mathcal{F}(\eta_{\ell_n}) \xrightarrow[a.e.]{n\to\infty} \mathcal{F}(\psi)$ and $\mathcal{F}(\eta_{\ell_n}') \xrightarrow[a.e.]{n\to\infty} \mathcal{F}(\psi')$.[a] In particular, for a.e. $p \in \mathbb{R}$ we have

$$\mathcal{F}(\psi')(p) = \lim_{n\to\infty} \mathcal{F}(\eta_{\ell_n}')(p) = \lim_{n\to\infty} ip\mathcal{F}(\eta_{\ell_n})(p) = ip\mathcal{F}(\psi)(p).$$

The claim follows.

Now we have for almost every $p \in \mathbb{R}$

$$\mathcal{F}(P\psi)(p) = \mathcal{F}(\tfrac{1}{i}\psi')(p) = \tfrac{1}{i}\mathcal{F}(\psi')(p) = \tfrac{1}{i}(ip\mathcal{F}(\psi)(p)) = p\mathcal{F}(\psi)(p) \tag{12}$$

Since $P\psi \in L^2(\mathbb{R};\mathbb{C})$ we have $\mathcal{F}(P\psi) \in L^2(\mathbb{R};\mathbb{C})$ and thus

$$\infty > \int_{\mathbb{R}} |\mathcal{F}(P\psi)(p)|^2 \,\mathrm{d}p = \int_{\mathbb{R}} |p\mathcal{F}(\psi)(p)|^2 \,\mathrm{d}p = \int_{\mathbb{R}} |p|^2 |\mathcal{F}(\psi)(p)|^2 \,\mathrm{d}p.$$

This yields by Definition 2.0.1 that $\mathcal{F}(\psi) \in D(Q)$. Futhermore we have for a.e. $p \in \mathbb{R}$

$$(Q\mathcal{F}(\psi))(p) = p\mathcal{F}(\psi)(p) \underset{(12)}{=} \mathcal{F}(P\psi)(p),$$

so that $\mathcal{F}P(\psi) = Q\mathcal{F}(\psi)$. Applying $\mathcal{F}^{-1} : L^2(\mathbb{R};\mathbb{C}) \to L^2(\mathbb{R};\mathbb{C})$ on both sides yields the claim.

[a] Here, "$\xrightarrow[a.e.]{n\to\infty}$" stands for convergence pointwise almost everywhere

This is what we mean by saying *after Fourier transform*, P and Q play the same role. Given that this is so, the following formula for the expectation of the momentum operator P will not come as a surprise – it looks precisely like Formula (3) for the expectation of Q, which we recall here for convenience:

$$\mu_\psi(Q) = \int_{\mathbb{R}} x|\psi(x)|^2 \, \mathrm{d}x \qquad \text{for all } \psi \in D(Q). \tag{13}$$

The only difference is that it has to be formulated in the Fourier image.

Proposition 2.2.12

Suppose that $\psi \in D(P)$ and $\hat{\psi} := \mathcal{F}(\psi)$. Then

$$\mu_\psi(P) = \mu_{\hat{\psi}}(Q) = \int_{\mathbb{R}} p|\hat{\psi}(p)|^2 \, \mathrm{d}p. \tag{14}$$

Before we prove this formula we would also like to discuss its interpretation as an expectation. If $\psi \in L^2(\mathbb{R}; \mathbb{C})$ is such that $\int_{\mathbb{R}} |\psi(x)|^2 \, \mathrm{d}x = 1$ we have by unitariness of the Fourier transform

$$\int_{\mathbb{R}} |\hat{\psi}(p)|^2 \, \mathrm{d}p = \int_{\mathbb{R}} |\psi(x)|^2 \, \mathrm{d}x = 1,$$

so that $p \mapsto |\hat{\psi}(p)|^2$ is also a probability density. The right hand side of (14) is nothing but the expectation of the distribution associated to this density.

Proof. Let $\psi \in D(P) = W^{1,2}(\mathbb{R}; \mathbb{C})$. Recall from Proposition 2.2.11 that $\hat{\psi} = \mathcal{F}(\psi) \in D(Q)$.

Intermediate claim For each $f, g \in L^2(\mathbb{R}; \mathbb{C})$ we have $\langle \mathcal{F}(f), \mathcal{F}(g) \rangle = \langle f, g \rangle$.

This is actually a direct consequence of linearity and the unitariness of the Fourier transform. Indeed, standard computations with properties of the scalar product show that for any $f, g \in L^2(\mathbb{R}; \mathbb{C})$ we have

$$2\mathrm{Re}\langle f, g \rangle = \|f + g\|_{L^2}^2 - \|f\|_{L^2}^2 - \|g\|_{L^2}^2,$$

Using this with $\mathcal{F}(f)$ instead of f and $\mathcal{F}(g)$ instead of g we may compute

$$\begin{aligned} 2\mathrm{Re}\langle \mathcal{F}(f), \mathcal{F}(g) \rangle &= \|\mathcal{F}(f) + \mathcal{F}(g)\|_{L^2}^2 - \|\mathcal{F}(f)\|_{L^2}^2 - \|\mathcal{F}(g)\|_{L^2}^2 \\ &= \|\mathcal{F}(f + g)\|_{L^2}^2 - \|\mathcal{F}(f)\|_{L^2}^2 - \|\mathcal{F}(g)\|_{L^2}^2 \\ &= \|f + g\|_{L^2}^2 - \|f\|_{L^2}^2 - \|g\|_{L^2}^2 = 2\mathrm{Re}\langle f, g \rangle. \end{aligned}$$

We infer $\mathrm{Re}\langle \mathcal{F}(f), \mathcal{F}(g) \rangle = \mathrm{Re}\langle f, g \rangle$. Repeating the same computation with if instead of f we can also obtain obtain $\mathrm{Im}\langle \mathcal{F}(f), \mathcal{F}(g) \rangle = \mathrm{Im}\langle f, g \rangle$. The claim follows.

Using the intermediate claim and Proposition 2.2.11 we infer

$$\begin{aligned}\mu_\psi(P) &= \langle P\psi, \psi\rangle = \langle \mathcal{F}(P\psi), \mathcal{F}(\psi)\rangle \\ &\underset{\text{Prop2.2.11}}{=\!=\!=} \langle Q\mathcal{F}(\psi), \mathcal{F}(\psi)\rangle = \langle Q\hat{\psi}, \hat{\psi}\rangle = \mu_{\hat{\psi}}(Q) \underset{(13)}{=} \int_{\mathbb{R}} p|\hat{\psi}(p)|^2 \,\mathrm{d}p,\end{aligned}$$

where we have used in the second to last step also that according to Proposition 2.2.11 we have $\hat{\psi} \in D(Q)$.

Similar formulas can be proved for the variance of the momentum. We refer to the exercises and shall not go deeper right now. What I would however like to convey is the following conclusion

Conclusion. The formula $P = \mathcal{F}^{-1}Q\mathcal{F}$ signifies that the Fourier transform allows a transition between position space and momentum space. All the probabilistic quantities of Q (expectation, variance) that are computed with the probability density $|\psi|^2$ can be computed in the same way for P, but with the probability density $|\hat{\psi}|^2$.

3 The Schrödinger equation

In the previous chapters our given physical system was a single particle on the real line $\mathbb{R}$. Since time has not played a role, we have considered the whole system only at a given point in time t_0. From now on we would like to describe, how the particle *evolves in time*. Also, we will from now on not only look at particles on $\mathbb{R}$ but on $\mathbb{R}^d$. For this reason we have now a space variable $x = (x_1, ..., x_d) \in \mathbb{R}^d$ with multiple components. Let us briefly summarize the physical situation

- At time $t = 0$ our particle has an *initial state function* $\psi_0 \in L^2(\mathbb{R}^d; \mathbb{C})$ with $\int_{\mathbb{R}^d} |\psi_0(x)|^2 \, \mathrm{d}x = 1$
- The evolution of the particle in time is influenced by
  - The quantum nature of the particle (i.e. one needs to formulate a law that somehow reflects the wave property of the particle)
  - Some external forces, i.e. we assume that the particle lives in a *potential landscape* with potential $V : \mathbb{R}^d \to \mathbb{R}$ (e.g. if gravitational forces apply we would have $V(x_1, ..., x_d) = mgx_d$)

Again, we can only make probabilistic statements about particles so we again seek to describe the (now time-dependent!) state function $\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$, $\psi = \psi(t, x_1, ..., x_d)$.
It turns out that the evolution law we need to describe this state function is the *Schrödinger equation*. Actually, that ψ evolves according to the Schrödinger equation is an *axiom*. So in particular it is nothing that we can prove, but something that we take for granted and develop the whole theory on this basis. Given that the theory is very successful and its predictions can be verified in experiments, this should be enough justification for the Schrödinger equation. It will however take us some time to understand what the Schrödigner equation actually means. The reason for that is that if one look into the standard literature, the Schrödinger equation involve derivatives. However, so far we have not specified any regularity of ψ and we actually can't because we would like to allow also very rough initial data $\psi_0 \in L^2(\mathbb{R}^d; \mathbb{C})$, which do not have derivatives in the classical sense.
This brings into play the insights of Part I of the lecture, where we have learned to take derivates of irregular objects — with distribution theory we will be able to understand the Schrödinger equation thoroughly.
For a first formulation however we have to be *unmathematical* and just write down the equation.

Axiom 3.0.1 — Schrödinger Equation

Let $V : \mathbb{R}^d \to \mathbb{R}$. The dynamics of a particle with state function $\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$ throughout time is given by the *Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi(t, x) = -\frac{1}{2}\Delta_x\psi(t, x) + V(x)\psi(t, x), \tag{15}$$

where $\Delta_x = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$ denotes the Laplace operator in the spatial variables. As a shorthand notation we introduce the operator $H = -\frac{1}{2}\Delta_x + V\mathrm{Id}$ and rewrite $i\frac{\partial}{\partial t}\psi = H\psi$.

The goal of this chapter will be to discuss how we can really understand this equation (even for irregular state functions and potentials, which can sometimes occur – already as an initial value at time $t = 0$ we have to admit them). Mathematical questions that arise naturally are

- **Initial value problems.** Let's say we have some initial state $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. In which sense does there exist a solution of (15) that satisfies $\psi(0,\cdot) = \psi_0$? Do special conditions on ψ_0 have to be required?
- **Square integrability.** The above solution only represents a meaningful state function if $\psi(t,\cdot) \in L^2(\mathbb{R}^d;\mathbb{C})$ (and even $\|\psi(t,\cdot)\|_{L^2} = 1$). Is this always ensured?
- **Long time behavior.** How do solutions behave for large times? What can be said about *asympotics* of solutions?

We will briefly outline how these points are adressed in physics literature. Let us have a closer look at the second point. If for some $t > 0$ the function $\psi(t,\cdot)$ is a meaningful state function then we would have

$$\int_{\mathbb{R}^d} |\psi(t,x)|^2 \,\mathrm{d}x = 1.$$

In particular, the map $t \mapsto \|\psi(t,\cdot)\|_{L^2}$ must be constant (and equal to 1). If ψ were regular enough, this would follow by an easy computation which we show at this point without any justification

$$\begin{aligned}
\frac{d}{dt}\int_{\mathbb{R}^d} |\psi(t,x)|^2 \,\mathrm{d}x &= \frac{d}{dt}\int_{\mathbb{R}^d} \psi(t,x)\overline{\psi(t,x)} \,\mathrm{d}x \\
&= \int_{\mathbb{R}^d} \left(\frac{\partial}{\partial t}\psi(t,x)\overline{\psi(t,x)} + \psi(t,x)\overline{\frac{\partial}{\partial t}\psi(t,x)}\right) \,\mathrm{d}x \\
&= \int_{\mathbb{R}^d} 2\mathrm{Re}\left(\frac{\partial}{\partial t}\psi(t,x)\overline{\psi(t,x)}\right) \,\mathrm{d}x = 2\mathrm{Re}\int_{\mathbb{R}^d} \frac{\partial}{\partial t}\psi(t,x)\overline{\psi(t,x)} \,\mathrm{d}x \\
&= 2\mathrm{Re}\int_{\mathbb{R}^d} \left(\frac{i}{2}\Delta_x\psi(t,x) - iV(x)\psi(t,x)\right)\overline{\psi(t,x)} \,\mathrm{d}x \\
&= 2\mathrm{Re}\left(\frac{i}{2}\int_{\mathbb{R}^d} \Delta_x\psi(t,x)\overline{\psi(t,x)} \,\mathrm{d}x - i\int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2 \,\mathrm{d}x\right) \qquad (16)
\end{aligned}$$

The last summand obviously has real part zero as V is real-valued and thus the number appearing there is purely imaginary. In the first part we can integrate by parts and (assuming that we are allowed to do so without boundary parts) we may rewrite

$$\frac{i}{2}\int_{\mathbb{R}^d} \Delta_x\psi(t,x)\overline{\psi(t,x)} \,\mathrm{d}x = -\frac{i}{2}\int_{\mathbb{R}^d} \nabla_x\psi(t,x)\cdot\overline{\nabla_x\psi(t,x)} \,\mathrm{d}x = -\frac{i}{2}\int_{\mathbb{R}^d} |\nabla_x\psi(t,x)|^2 \,\mathrm{d}x,$$

which is also purely imaginary. Using this in (16) yields $\frac{d}{dt}\int_{\mathbb{R}^d} |\psi(t,x)|^2 \,\mathrm{d}x = 0$. The derivation however has quite some mathematical flaws

- We do not know if we are allowed to interchange derivative and integral in the first step.
- We would like to think about ψ as some irregular L^2-function and we do not know for which t, x $(t,x) \mapsto \psi(t,x)$ possesses derivatives in the classical sense.
- We have integrated by parts without boundary terms. Is this really justified?

All of these questions can not be answered before making appropriate sense of how one is supposed to read the equation for irregular initial data $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. We will pursue this in the coming chapters.

3.1 The free Schrödinger equation

To make sense of the above equation we first focus on the simplest possible case, that is $V \equiv 0$ (i.e. a *free particle*). In particular, the Schrödinger equation takes the form

$$i\frac{\partial}{\partial t}\psi(t,x) + \frac{1}{2}\Delta_x\psi(t,x) = 0. \tag{17}$$

The operator $T = i\partial_t + \frac{1}{2}\Delta_x$ has constant coefficients, which means that it must possess a fundamental solution (see Theorem 9.2 in Part II of the lecture). We will also determine this fundamental solution subsequently. To develop an understanding of (17) we first look see what happens with smooth solutions. Assume for the moment that ψ is smooth in t and x and $\psi(t,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ for all $t \in \mathbb{R}$. Moreover we define $\psi_0 := \psi(0,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. We may then form the *Fourier transform* in the x-Variable

$$\hat{\psi}(t,p) := \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x, \tag{18}$$

where $p = (p_1,...,p_d) \in \mathbb{R}^d$. If we further assume that $\frac{\partial}{\partial t}\psi(t,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we may switch time derivative and integral (Left to the reader as an exercise!). We compute for $t \in \mathbb{R}$ and $p \in \mathbb{R}^d$

$$i\frac{\partial}{\partial t}\hat{\psi}(t,p) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} i\frac{\partial}{\partial t}\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x \tag{19}$$

Using the Schrödinger equation in (19) and integrations by parts this yields

$$\begin{aligned}
i\frac{\partial}{\partial t}\hat{\psi}(t,p) &= -\frac{1}{2}\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\Delta_x\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x = -\frac{1}{2}\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\sum_{i=1}^d\frac{\partial^2}{\partial x_i^2}\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x \\
&= -\frac{1}{2}\frac{1}{(2\pi)^{\frac{d}{2}}}\sum_{i=1}^d\int_{\mathbb{R}^d}\frac{\partial^2}{\partial x_i^2}\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x = -\frac{1}{2}\frac{1}{(2\pi)^{\frac{d}{2}}}\sum_{i=1}^d\int_{\mathbb{R}^d}\psi(t,x)\frac{\partial^2}{\partial x_i^2}e^{-ip\cdot x}\,\mathrm{d}x \\
&= -\frac{1}{2}\frac{1}{(2\pi)^{\frac{d}{2}}}\sum_{i=1}^d\int_{\mathbb{R}^d}\psi(t,x)(-i)^2p_i^2e^{-ip\cdot x}\,\mathrm{d}x = \frac{1}{2}\frac{1}{(2\pi)^{\frac{d}{2}}}\sum_{i=1}^d p_i^2\int_{\mathbb{R}^d}\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x \\
&= \frac{1}{2}|p|^2\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\psi(t,x)e^{-ip\cdot x}\,\mathrm{d}x = \frac{1}{2}|p|^2\hat{\psi}(t,p).
\end{aligned}$$

Multiplying by $-i$ we obtain

$$\frac{\partial}{\partial t}\hat{\psi}(t,p) = -\frac{i}{2}|p|^2\hat{\psi}(t,p)$$

If one fixes some $p \in \mathbb{R}^d$, this yields an ODE for $f(t) := \hat{\psi}(t,p)$, namely $f'(t) = -\frac{i}{2}|p|^2 f(t)$. Each solution of this is given by $f(t) = ce^{-\frac{i}{2}|p|^2 t}$ for some $c \in \mathbb{R}$.[1] We obtain

$$\hat{\psi}(t,p) = ce^{-\frac{i}{2}|p|^2 t}. \tag{20}$$

The constant c can easily be found when looking at $t = 0$. Indeed, for $t = 0$ the right hand side yields c and the left hand side yields

$$\hat{\psi}(0,p) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}} \psi(0,x)e^{-ip\cdot x}\,\mathrm{d}x = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}} \psi_0(x)e^{-ip\cdot x}\,\mathrm{d}x = \mathcal{F}(\psi_0)$$

Therefore, (20) yields

$$\hat{\psi}(t,p) = e^{-\frac{i}{2}|p|^2 t}\mathcal{F}(\psi_0)(p).$$

Recall that $\hat{\psi}(t,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Hence we can apply the backtansform $\mathcal{F}^{-1}$ to retrieve the original function ψ. More precisely

$$\psi(t,\cdot) = \mathcal{F}^{-1}\left(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)\right). \tag{21}$$

If one inspects these calculations more closely we see that we have shown

Proposition 3.1.1 — Solutions for Initial-Data in $\mathcal{S}$

Let $\psi_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Then there exists a smooth solution $\psi : \mathbb{R}\times\mathbb{R}^d \to \mathbb{C}$ to (17) that satisfies $\psi(0,\cdot) = \psi_0$ and $\psi(t,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$, $\frac{\partial}{\partial t}\psi(t,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ for all $t \in \mathbb{R}$. It is explicitly given by

$$\psi(t,x) = \mathcal{F}^{-1}\left(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)\right)(x)$$

The details are left as an exercise. The question we now would like to address is: Can we solve the Schrodinger equation for less regular initial data ψ_0? In order to address this question one could first observe that the expression on the right hand side of (21) makes sense even for less regular values of ψ_0. Indeed, if e.g. $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ then $\mathcal{F}(\psi_0) \in L^2(\mathbb{R}^d;\mathbb{C})$ and therefore $e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0) \in L^2(\mathbb{R}^d;\mathbb{C})$ for any $t \in \mathbb{R}$. This allows us to apply $\mathcal{F}^{-1}$ since $\mathcal{F}$ is a bijection on L^2 (cf. Theorem *a*). The big problem is that for $\psi_0 \in L^2$, $\Delta_x\psi_0$ does not make sense a a function and thus (17) can not make sense already at $t = 0$. And even if it would make sense

[1] For those who are not familiar with that: It its readily seen as follows. Suppose that $f \in C^\infty(\mathbb{R})$ satisfies $f'(t) = -\frac{i}{2}|p|^2 f(t)$ for all $t \in \mathbb{R}$. We define $g(t) := e^{\frac{i}{2}|p|^2 t}f(t)$ and compute that

$$g'(t) = \tfrac{i}{2}|p|^2 e^{\frac{i}{2}|p|^2 t}f(t) + e^{\frac{i}{2}|p|^2 t}f'(t) = \tfrac{i}{2}|p|^2 e^{\frac{i}{2}|p|^2 t}f(t) + e^{\frac{i}{2}|p|^2 t}(-\tfrac{i}{2}|p|^2 f(t)) = 0,$$

for all $t \in \mathbb{R}$ and obtain that g must be constant, i.e. $g(t) = c$ for some $c \in \mathbb{R}$. Now note that $f(t) = e^{-\frac{i}{2}|p|^2 t}g(t) = e^{-\frac{i}{2}|p|^2 t}c$ and conclude the claim.

the previous derivation can not be repeated as the representation formula (18) was used and this does not apply to all functions in L^2. How do we overcome these problems? The answer is: distributions!
Thankfully, we have already talked about derivatives in distributional sense and can also give a meaning to (17) if ψ is only a distribution. We shall do this in the next paragraph.

3.1.1 Distributional Solutions

We intend to give a meaning to (17) for distributions. Before we had for each $t \in \mathbb{R}$ a function $\psi(t, \cdot) \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$. Now, we would like for each $t \in \mathbb{R}$ a distribution $\psi_t \in \mathcal{S}'(\mathbb{R}^d; \mathbb{C})$. In particular, we view this now was a mapping $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d; \mathbb{C}), t \mapsto \psi_t$.

Definition 3.1.2 — Distributional solutions of the Schrödinger equation

We say that $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d; \mathbb{C}), t \mapsto \psi_t$ is a *distributional solution of the free Schrödinger equation* if for all $\varphi \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ the map $t \mapsto \psi_t(\varphi)$ is differentiable from $\mathbb{R}$ to $\mathbb{C}$ and for all $t \in \mathbb{R}$ we have

$$i\frac{d}{dt}\psi_t(\varphi) = -\frac{1}{2}(\Delta\psi_t)(\varphi) \qquad \text{for all } \varphi \in \mathcal{S}(\mathbb{R}^d; \mathbb{C}), \tag{22}$$

where $\Delta\psi_t$ denotes the distributional Laplacian of ψ_t, i.e. $(\Delta\psi_t)(\varphi) := \psi_t(\Delta\varphi)$.

Remark 3.1.3 — Continuity in Time

We would like to stress at this point that each distributional solution $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d; \mathbb{C})$ in the sense of Definition 3.1.2 is depends continuously on time. More precisely: If $(t_n)_{n\in\mathbb{N}} \subseteq \mathbb{R}$ is such that $t_n \xrightarrow[\mathbb{R}]{n\to\infty} t$, we have $\psi_{t_n} \xrightarrow[\mathcal{S}'(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_t$.

This is easily seen as follows: Let $t_n \xrightarrow[\mathbb{R}]{n\to\infty} t$. To show that $\psi_{t_n} \xrightarrow[\mathcal{S}'(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_t$ we must prove that for each $\varphi \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ we have $\psi_{t_n}(\varphi) \xrightarrow[\mathbb{C}]{n\to\infty} \psi_t(\varphi)$ $(*)$, see also Chapter 1.3.4 of part I of the lecture. However, since the map $t \mapsto \psi_t(\varphi)$ is differentiable, it must also be continuous. This implies $(*)$ directly.

In this section we prove the following theorem about the existence of distributional solutions

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Theorem 3.1.4 — Distributional solutions — Existence and Uniqueness

Let $\psi_0 \in \mathcal{S}'(\mathbb{R}^d; \mathbb{C})$. Then there exists a unique distributional solution $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d; \mathbb{C}), t \mapsto \psi_t$ of the free Schrödinger equation that attains the value ψ_0 at $t = 0$. It is given by the formula

$$\psi_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)) \qquad \text{for all } t \in \mathbb{R},$$

(this means that for each $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ and $t \in \mathbb{R}$ we have

$$\psi_t(\varphi) = \psi_0(\mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi))$$

Proof.

STEP 1. Existence.

Let $\psi_0 \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$. Define for $t \in \mathbb{R}$ the tempered distribution ψ_t via

$$\psi_t(\varphi) = \psi_0(\mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)) \quad \text{for all } \varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C}).$$

Next fix $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. It needs to be shown that $t \mapsto \psi_t(\varphi)$ is differentiable on $\mathbb{R}$ and (22) holds. Concerning first the differentiability we form for $h \in \mathbb{R}\backslash\{0\}$

$$\frac{\psi_{t+h}(\varphi) - \psi_t(\varphi)}{h} = \psi_0(\mathcal{F}^{-1}(\tfrac{e^{-\frac{i}{2}|\cdot|^2 h}-1}{h} e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi))$$

Now define $f_h : \mathbb{R}^d \to \mathbb{C}$ via $f_h(p) := \frac{e^{-\frac{i}{2}|p|^2 h}-1}{h}$. One readily checks that for each $\eta \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we have $f_h\eta \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{h\to 0} -\frac{i}{2}|\cdot|^2\eta$ as $h \to 0$. (Exercise!) Due to the fact that $\mathcal{F}^{-1}(\psi_0)$ is a tempered distribution (i.e. continuous with respect to $\mathcal{S}(\mathbb{R}^d;\mathbb{C})$-convergence) and that $\eta := e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)$ lies in $\mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we find

$$\lim_{h\to 0} \frac{\psi_{t+h}(\varphi) - \psi_t(\varphi)}{h} = \psi_0(\mathcal{F}^{-1}(-\tfrac{i}{2}|\cdot|^2 e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\varphi)),$$

which yields the differentiability of $t \mapsto \psi_t(\varphi)$ and

$$\frac{d}{dt}\psi_t(\varphi) = \psi_0(\mathcal{F}^{-1}(-\tfrac{i}{2}|\cdot|^2 e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\varphi)). \tag{23}$$

Moreover one readily checks that $-|p|^2\mathcal{F}\varphi(p) = \mathcal{F}(\Delta\varphi)(p)$ for all $p \in \mathbb{R}^n$ (this is a straightforward consequence of Remark 2.2.8 since $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ is a Schwartz function). This and (23) yield

$$\frac{d}{dt}\psi_t(\varphi) = \frac{i}{2}\psi_0(\mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\Delta\varphi)) = \frac{i}{2}\psi_t(\Delta\varphi) = \frac{i}{2}(\Delta\psi_t)(\varphi).$$

Multiplying with i implies

$$i\frac{d}{dt}\psi_t(\varphi) = -\frac{1}{2}(\Delta\psi_t)(\varphi).$$

Existence is shown.

STEP 2. Uniqueness.

If we have two solutions with the same initial value ψ_0 we can subtract them from each other and obtain a solution with initial value $0 \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$. All we now have to show is that each distributional solution $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ with initial value $\psi_0 = 0$ vanishes identically. Let $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d;\mathbb{C}), t \mapsto \psi_t$ be such a solution.

Intermediate Claim. Let $\tau \in \mathbb{R}$ and $\theta \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Then there exists a smooth function $\eta : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$ such that η solves the so-called *adjoint equation* $\begin{cases} i\frac{\partial}{\partial t}\eta(t,x) = +\frac{1}{2}\Delta\eta(t,x) & t \in \mathbb{R}, x \in \mathbb{R}^d \\ \eta(\tau,\cdot) = \theta \end{cases}$. Moreover, for each $t \in \mathbb{R}$ we have $\eta(t,\cdot), \frac{\partial}{\partial t}\eta(t,\cdot) \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Furthermore, for each $t \in \mathbb{R}$ there holds $\frac{\eta(t+h,\cdot)-\eta(t,\cdot)}{h} \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{h\to 0} \frac{\partial\eta}{\partial t}(t,\cdot)$. Furthermore we have $\frac{\eta(t+h,\cdot)-\eta(t,\cdot)}{h} \xrightarrow{\mathcal{S}(\mathbb{R}^d;\mathbb{C})} \frac{\partial\eta}{\partial t}$ as $h \to 0$ and $\frac{\partial\eta}{\partial t}(t+h,\cdot) \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{h\to 0} \frac{\partial\eta}{\partial t}(t,\cdot)$.

This intermediate claim is readily established. Indeed, one can define

$$\eta : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}, \eta(t,x) := \mathcal{F}^{-1}(e^{\frac{i}{2}|\cdot|^2(t-\tau)}\mathcal{F}\theta)(x)$$

and easily calculate that this has all the desired properties (tedious but all doable, compare also to exercise sheet 2 question 2).

We now wish to calculate $\frac{d}{dt}\psi_t(\eta(t,\cdot))$. This is nontrivial since we now have to dependencies on t. To this end we observe that for $h \in \mathbb{R}\backslash\{0\}$

$$\frac{\psi_{t+h}(\eta(t+h,\cdot)) - \psi_t(\eta(t,\cdot))}{h} = \frac{\psi_{t+h}(\eta(t,\cdot)) - \psi_t(\eta(t,\cdot))}{h} + \psi_{t+h}\left(\frac{\eta(t+h,\cdot) - \eta(t,\cdot)}{h}\right). \tag{24}$$

We now discuss the behavior of both summands in (24) separately.

(1) First summand in (24).

Letting $h \to 0$ the first summand tends to $(\frac{d}{dt}\psi_t)(\eta(t,\cdot)) = \frac{i}{2}\psi_t(\Delta\eta(t,\cdot))$, where we have used the distributional Schrödinger equation in the last step.

(2) Second summand in (24).

The behavior of the second summand is not so easy to study since we have still two dependencies on h. We will however be able to do this with Lemma 3.1.5 (see below, a refinement of Theorem 1.3.7. in Part I of the lecture). Let $(h_n)_{n\in\mathbb{N}}$ be any sequence that converges to 0 and define $L_n := \psi_{t+h_n} \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ and $\varphi_n := \frac{\eta(t+h_n,\cdot)-\eta(t,\cdot)}{h_n}$. To check the prerequisites of Lemma 3.1.5 we fix some arbitrary $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ and form $\sup_{n\in\mathbb{N}} |L_n\varphi| = \sup_{n\in\mathbb{N}} |\psi_{t+h_n}(\varphi)|$. Now, since $(t+h_n)_{n\in\mathbb{N}}$ is a bounded sequence we find some $K \subset \mathbb{R}$ compact such that $(t+h_n)_{n\in\mathbb{N}} \subseteq K$ Since $t \mapsto \psi_t(\varphi)$ is a differentiable (and thus continuous) we obtain $\sup_{n\in\mathbb{N}} |\psi_{t+h_n}(\varphi)| \leqslant \sup_{t'\in K} |\psi_{t'}(\varphi)| < \infty$, since continuous functions attain maxima on compact sets. Now recall from Remark 3.1.3 that $L_n = \psi_{t+h_n} \xrightarrow[\mathcal{S}'(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_t =: L$ and from the intermediate claim that $\varphi_n = \frac{\eta(t+h_n,\cdot)-\eta(t,\cdot)}{h_n} \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \frac{\partial\eta}{\partial t}(t,\cdot) =: \varphi$. Lemma 3.1.5 therefore applies and yields

$$\lim_{n\to\infty} \psi_{t+h_n}\left(\frac{\eta(t+h_n,\cdot)-\eta(t,\cdot)}{h_n}\right) = \lim_{n\to\infty} L_n\varphi_n = L\varphi = \psi_t(\tfrac{\partial\eta}{\partial t}(t,\cdot)).$$

Since $(h_n)_{n\in\mathbb{N}}, h_n \xrightarrow{n\to\infty} 0$ was arbitrary we obtain

$$\lim_{h\to 0} \psi_{t+h}\left(\frac{\eta(t+h,\cdot)-\eta(t,\cdot)}{h}\right) = \psi_t(\tfrac{\partial\eta}{\partial t}(t,\cdot)).$$

(3) Passage to the limit in (24).

We can now finally pass to the limit in both summands of (24) and obtain

$$\frac{d}{dt}\psi_t(\eta(t,\cdot)) = \tfrac{i}{2}\psi_t(\Delta\eta(t,\cdot)) + \psi_t(\tfrac{\partial}{\partial t}\eta(t,\cdot)).$$

The intermediate claim implies that $\frac{\partial}{\partial t}\eta(t,\cdot) = -\frac{i}{2}\Delta\eta(t,\cdot)$, so that

$$\frac{d}{dt}\psi_t(\eta(t,\cdot)) = \tfrac{i}{2}\psi_t(\Delta\eta(t,\cdot)) + \psi_t(-\tfrac{i}{2}\Delta\eta(t,\cdot)) = 0,$$

by linearity of ψ_t. Hence $t \mapsto \psi_t(\eta(t,\cdot))$ is constant. Note that due to the fact that $\psi_0 = 0$ we have that at $t = 0$ the value zero is attained and we conclude

$$\forall t \in \mathbb{R}: \qquad \psi_t(\eta(t,\cdot)) = 0.$$

Now we look at the value $t = \tau$ and conclude

$$0 = \psi_\tau(\eta(\tau,\cdot)) = \psi_\tau(\theta).$$

Since $\theta \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ was arbitrary we conclude that $\psi_\tau = 0$ (as a tempered distibution). Since also $\tau \in \mathbb{R}$ was arbitrary we conclude that $\psi \equiv 0$. Uniqueness is shown.

The above proof has used the following lemma which we state for the sake of completeness.

Lemma 3.1.5

Let $(L_n)_{n\in\mathbb{N}} \subset \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ be a sequence of tempered distributions and $(\varphi_n)_{n\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Further let $L \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ and $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Then if $L_n \xrightarrow[\mathcal{S}'(\mathbb{R}^d;\mathbb{C})]{n\to\infty} L$ and $\varphi_n \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$, we have $L_n\varphi_n \xrightarrow[\mathbb{C}]{n\to\infty} L\varphi$ as $n\to\infty$

Proof. Let $(L_n)_{n\in\mathbb{N}}, (\varphi_n)_{n\in\mathbb{N}}, L, \varphi$ be as in the statement. Before we start the proof we would like to mention the following fact. Since for each $\eta \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we have $L_n\eta \xrightarrow{n\to\infty} L\eta$ we have

$$\forall \eta \in \mathcal{S}(\mathbb{R}^d;\mathbb{C}): \qquad \sup_{n\in\mathbb{N}} |L_n\eta| < \infty. \tag{25}$$

The rest of the proof is subdivided in two steps.

Step 1. We first prove the claim for $\varphi = 0$. In particular we need to prove $L_n\varphi_n \xrightarrow[\mathbb{C}]{n\to\infty} 0$ as $n\to\infty$.

Assume the opposite, then one can find a subsequence $(m_n)\subseteq\mathbb{N}$ and $c>0$ such that $|L_{m_n}\varphi_{m_n}| \geqslant c$ for all $n\in\mathbb{N}$. To make notation simpler we redefine in the following $L_n = L_{m_n}$ and $\varphi_n = \varphi_{m_n}$ (with slight abuse of notation). In particular, there exists $c>0$ such that

$$|L_n\varphi_n| \geqslant c \qquad \forall n\in\mathbb{N}. \tag{26}$$

Since $\varphi_n \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$ we have for each multiindex[a] α and $m\in\mathbb{N}$

$$\sup_{x\in\mathbb{R}^d} |x|^m |D^\alpha\varphi_n(x)| \xrightarrow{n\to\infty} 0.$$

In particular we find $(\ell_n^{(1)})_{n\in\mathbb{N}}\subseteq\mathbb{N}$ such that for all multiindices α with[b] $|\alpha|\leqslant 1$ we have

$$\sup_{x\in\mathbb{R}^d}(1+|x|)|D^\alpha\varphi_{\ell_n^{(1)}}(x)| \leqslant \frac{1}{4^n}$$

We further find a subsequence $(\ell_n^{(2)})_{n\in\mathbb{N}}\subseteq(\ell_n^{(1)})_{n\in\mathbb{N}}$ such that for all multiindices α with $|\alpha|\leqslant 2$ we have

$$\sup_{x\in\mathbb{R}^d}(1+|x|)^2|D^\alpha\varphi_{\ell_n^{(2)}}(x)| \leqslant \frac{1}{4^n}$$

This yields nested subsequences $(\ell_n^{(m)})_{n\in\mathbb{N}}\subseteq(\ell_n^{(m-1)})_{n\in\mathbb{N}}\subseteq \dots \subseteq (\ell_n^{(1)})_{n\in N}$ with the property

$$\sup_{|\alpha|\leqslant m}\sup_{x\in\mathbb{R}^d}(1+|x|^m)|D^\alpha\varphi_{\ell_n^{(m)}}(x)| \leqslant \frac{1}{4^n}$$

Using a diagonal trick, i.e. considering $\ell_n := \ell_n^{(n)}$ we can find a subsequence $(\ell_n)_{n\in\mathbb{N}}$ such that for all $n\in\mathbb{N}$

$$\sup_{|\alpha|\leqslant n}\sup_{x\in\mathbb{R}^d}(1+|x|)^n|D^\alpha\varphi_{\ell_n}(x)| \leqslant \frac{1}{4^n}.$$

Now define $\psi_{\ell_n} := 2^n \varphi_{\ell_n}$. Then

$$\sup_{|\alpha|\leqslant n} \sup_{x\in\mathbb{R}^d} (1+|x|)^n |D^\alpha \psi_{\ell_n}(x)| \leqslant \frac{1}{2^n}. \tag{27}$$

In particular $\psi_{\ell_n} \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$. Moreover, by (26) we have $|L_{\ell_n}\psi_{\ell_n}| \xrightarrow{n\to\infty} \infty$ $(*)$. For $n \in \mathbb{N}$ define also $c_n := \sup_{m\in\mathbb{N}} |L_m \psi_{\ell_n}|$ (which is finite due to (25)). Now choose $k_1 > 1$ such that

- $|L_{\ell_{k_1}}\psi_{\ell_{k_1}}| > c_1 + 1 + 1$ (which can be found due to $(*)$) and
- $|L_{\ell_1}\psi_{\ell_{k_1}}| < \frac{1}{2}$ (which can be achieved since $\psi_n \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$).

Next choose $k_2 > k_1$ such that

- $|L_{\ell_{k_2}}\psi_{\ell_{k_2}}| > c_1 + c_{k_1} + 2 + 1$ (which can be found due to $(*)$ and
- $|L_{\ell_1}\psi_{\ell_{k_2}}| < \frac{1}{4}$ and $|L_{\ell_{k_1}}\psi_{\ell_{k_2}}| < \frac{1}{2}$ (which can be achieved since $\psi_n \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$).

Next choose $k_3 > k_2$ such that

- $|L_{\ell_{k_3}}\psi_{\ell_{k_3}}| > c_1 + c_{k_1} + c_{k_2} + 3 + 1$ (which can be found due to $(*)$ and
- $|L_{\ell_1}\psi_{\ell_{k_3}}| < \frac{1}{8}$ and $|L_{\ell_{k_1}}\psi_{\ell_{k_3}}| < \frac{1}{4}$ and $|L_{\ell_{k_2}}\psi_{\ell_{k_3}}| < \frac{1}{2}$ (which can be achieved since $\psi_n \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$).

Inductively obtain a subsequence $(k_n)_{n\in\mathbb{N}_0}$, such that $k_0 = 1$ and

$$\begin{aligned} &\text{(I)} \qquad |L_{\ell_{k_n}}\psi_{\ell_{k_n}}| \geqslant \sum_{j=1}^{n-1} c_{k_j} + n + 1, \\ &\text{(II)} \qquad \forall j = 1, ..., n-1: \quad |L_{\ell_{k_j}}\psi_{\ell_{k_n}}| \leqslant \frac{1}{2^{n-j}} \end{aligned} \tag{28}$$

Next define

$$\psi := \sum_{m\geqslant 1} \psi_{\ell_{k_m}}$$

We leave it as an exercise to show that this series converges and $\psi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ (this is based on (27)). Moreover we leave it as an excercise to show that $\sum_{m=1}^{s} \psi_{\ell_{k_m}} \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{s\to\infty} \psi$. As a result of this we obtain for any $n \in \mathbb{N}$

$$L_{\ell_{k_n}}(\psi) = \sum_{m=1}^{\infty} L_{\ell_{k_n}}(\psi_{\ell_{k_m}}) = \sum_{m=1}^{n-1} L_{\ell_{k_n}}(\psi_{\ell_{k_m}}) + L_{\ell_{k_n}}(\psi_{\ell_{k_n}}) + \sum_{m=n+1}^{\infty} L_{\ell_{k_n}}(\psi_{\ell_{k_m}}) \tag{29}$$

Now (II) in (28) yields

$$\sum_{m=n+1}^{\infty} |L_{\ell_{k_n}}(\psi_{\ell_{k_m}})| \leqslant \sum_{m=n+1}^{\infty} \frac{1}{2^{m-n}} = \sum_{m=1}^{\infty} \frac{1}{2^m} = 1.$$

This and the inverse triangle inequality in (29) yield

$$\begin{aligned} |L_{\ell_{k_n}}(\psi)| &\geqslant |L_{\ell_{k_n}}(\psi_{\ell_{k_n}})| - \sum_{m=1}^{n-1} |L_{\ell_{k_n}}(\psi_{\ell_{k_m}})| - \sum_{m=n+1}^{\infty} |L_{\ell_{k_n}}(\psi_{\ell_{k_m}})| \\ &\geqslant |L_{\ell_{k_n}}(\psi_{\ell_{k_n}})| - \sum_{m=1}^{n-1} |L_{\ell_{k_n}}(\psi_{\ell_{k_m}})| - 1. \end{aligned} \tag{30}$$

Now note that due to (I) in (28) and the definition of c_n we have

$$|L_{\ell_{k_n}}\psi_{\ell_{k_n}}| \geqslant \sum_{j=1}^{n-1} c_{k_j} + n + 1 \geqslant \sum_{j=1}^{n-1} |L_{\ell_{k_n}}(\psi_{\ell_{k_j}})| + n + 1$$

Using this in (30) we obtain

$$|L_{\ell_{k_n}}(\psi)| \geqslant \sum_{j=1}^{n-1} |L_{\ell_{k_n}}(\psi_{\ell_{k_j}})| + n + 1 - \sum_{m=1}^{n-1} |L_{\ell_{k_n}}(\psi_{\ell_{k_m}})| - 1 = n.$$

This yields in particular that $\sup_{k\in\mathbb{N}} |L_k\psi| = \infty$, contradicting (25).

Step 2. We now show the claim for general φ.

Suppose that $\varphi_n \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$. Then $\varphi_n - \varphi \xrightarrow[\mathcal{S}(\mathbb{R}^d;\mathbb{C})]{n\to\infty} 0$. Step 1 implies

$$L_n(\varphi_n - \varphi) \xrightarrow[\mathbb{C}]{n\to\infty} L(0) = 0 \tag{31}$$

Now

$$L_n\varphi_n - L\varphi = L_n\varphi_n - L_n\varphi + L_n\varphi - L\varphi = L_n(\varphi_n - \varphi) + [L_n\varphi - L\varphi].$$

The first summand converges to zero by (31). The last summand converges to zero as $L_n \xrightarrow[\mathcal{S}'(\mathbb{R}^d;\mathbb{C})]{n\to\infty} L$.

[a] A multiindex is a vector in $\mathbb{N}_0^d$. For $\alpha = (\alpha_1, ..., \alpha_d$ and $f \in C^\infty(\mathbb{R}^d)$ we set $D^\alpha f := \partial_1^{\alpha_1} ... \partial_d^{\alpha_d} f$.
[b] For a multiindex $\alpha \in \mathbb{N}_0^d$ we set $|\alpha| := \alpha_1 + ... + \alpha_d$

3.1.1.1 Square integrability We have now discussed how initial value problems for irregular initial values can be understood — even for initial values $\psi_0 \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ and not just in $L^2(\mathbb{R}^d;\mathbb{C})$. Since however only functions in $L^2(\mathbb{R}^d;\mathbb{C})$ are physical we will be relieved after deriving the following proposition

Proposition 3.1.6 — Square Integrability

Let $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ and let $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution of the free Schrödinger equation with initial datum ψ_0 (interpreted as a tempered distribution by means of (9)). Then $\psi_t \in L^2(\mathbb{R}^d;\mathbb{C})$ for all $t \in \mathbb{R}$.[a]

[a] Rigorously speaking we should better say $\psi_t = L_f$ for some $f \in L^2(\mathbb{R}^d;\mathbb{C})$. We will leave this out for now and identify any $f \in L^2(\mathbb{R}^d;\mathbb{C})$ with its associated tempered distribution $L_f \in \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$ in the sense of (9). This way we have $L^2(\mathbb{R}^d;\mathbb{C}) \subseteq \mathcal{S}'(\mathbb{R}^d;\mathbb{C})$.

For this reason we will from now on often think about ψ as a map from $\mathbb{R}$ to $L^2(\mathbb{R}^d;\mathbb{C})$ and write $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C}))$ instead of $\psi : \mathbb{R} \to \mathcal{S}'(\mathbb{R}^d;\mathbb{C}))$ (but of course only provided that $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C}))$

Proof. We use the explicit formula in Theorem 3.1.4, that is

$$\psi_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)) \qquad \text{for all } t \in \mathbb{R}.$$

If $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$, then $\mathcal{F}(\psi_0) \in L^2(\mathbb{R}^d;\mathbb{C})$ (cf. Theorem a). Since for each $t \in \mathbb{R}$ and $p \in \mathbb{R}^d$ the complex number $e^{-\frac{i}{2}|p|^2 t}$ has complex absolute value 1, it is clear that for each $t \in \mathbb{R}$ also $e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)$ lies in $L^2(\mathbb{R}^d;\mathbb{C})$ for each $t \in \mathbb{R}$. Since also $\mathcal{F}^{-1}$ maps L^2-functions to L^2 functions we obtain for each $t \in \mathbb{R}$ that

$$\psi_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)) \in L^2(\mathbb{R}^d;\mathbb{C}).$$

The claim is shown.

We have now settled the question of existence and uniqueness for (distributional) solutions of the Schrödinger equation with initial data in $L^2(\mathbb{R}^d;\mathbb{C})$. The french mathematician Jacques Hadamard formulated in 1902 what is means for a problem to be *well-posed*. According to him, there are three properties that well-posed problems has to satisfy

(i) There exists a solution,

(ii) The solution has to be unique,

(iii) The solution depends *continuously* on the initial data.

Given that (i) and (ii) are settled for our problem, we now turn to (iii).

Proposition 3.1.7 — Continuous Dependence

Let $\psi_0, \tilde{\psi}_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. Let $\psi, \tilde{\psi} : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solutions to the free Schrödinger equation with initial values $\psi_0, \tilde{\psi}_0$ (respectively). Then for all $t \in \mathbb{R}$ we have

$$\|\psi_t - \tilde{\psi}_t\|_{L^2} = \|\psi_0 - \tilde{\psi}_0\|_{L^2}.$$

Proof. Again we use that for each $t \in \mathbb{R}$

$$\psi_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0)), \qquad \tilde{\psi}_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\tilde{\psi}_0)),$$

so that (by linearity of $\mathcal{F}, \mathcal{F}^{-1}$)

$$\psi_t - \tilde{\psi}_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0 - \tilde{\psi}_0)).$$

Using that $\mathcal{F}, \mathcal{F}^{-1}$ and the mutiplication with $e^{-\frac{i}{2}|\cdot|^2 t}$ are unitary[a] in $L^2(\mathbb{R}^d;\mathbb{C})$, we may compute

$$\|\psi_t - \tilde{\psi}_t\|_{L^2} = \|\mathcal{F}(\psi_t - \tilde{\psi}_t)\|_{L^2} = \|e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0 - \tilde{\psi}_0)\|_{L^2} = \|\mathcal{F}(\psi_0 - \tilde{\psi}_0)\|_{L^2} = \|\psi_0 - \tilde{\psi}_0\|_{L^2}.$$

[a] Here, a map $T : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is unitary if $\|Tf\|_{L^2} = \|f\|$ for all $f \in L^2(\mathbb{R}^d;\mathbb{C})$. That $\mathcal{F}, \mathcal{F}^{-1}$ are unitary follows from . For the multiplication operator we compute for any $f \in L^2(\mathbb{R}^d;\mathbb{C})$

$$\int_{\mathbb{R}^d} |e^{-\frac{i}{2}|p|^2 t} f(p)|^2 \,\mathrm{d}p = \int_{\mathbb{R}^d} |e^{-\frac{i}{2}|p|^2 t}|^2 \, |f(p)|^2 \,\mathrm{d}p = \int_{\mathbb{R}^d} |f(p)|^2 \,\mathrm{d}p$$

and infer that the multiplication with $e^{-\frac{i}{2}|\cdot|^2 t}|$ does not change the L^2-norm.

Remark 3.1.8

An important special case is $\tilde{\psi}_0 = 0$ (i.e. also $\tilde{\psi} = 0$)[a]. We conclude: If $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ is arbitrary and $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ is the unique distributional solution to the free Schrödinger equation with initial value ψ_0, then for all $t \in \mathbb{R}$ we have

$$\|\psi_t\|_{L^2} = \|\psi_0\|_{L^2}.$$

This is important since ψ_0 is a physical state function if and only if $\|\psi_0\|_{L^2} = 1$. The above formula states that in this case also ψ_t is a physical state function for all $t \in \mathbb{R}$. In particular we have now managed to replace the formal and unjustified computation in (16) by a rigorous argument.

[a] Note that this uses the uniqueness part in Theorem 3.1.4

Another question in the context of square integrability concerns attainment of the initial value ψ_0. Let $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ and let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution of the free Schrödinger equation with initial value ψ_0. We know from 3.1.3 that

$$\psi_t \xrightarrow{t\to 0} \psi_0 \qquad \text{in } \mathcal{S}'(\mathbb{R}^d;\mathbb{C}).$$

(Or, actually more precise $L_{\psi_t} \xrightarrow{t\to 0} L_{\psi_0}$ in $L^2(\mathbb{R}^d;\mathbb{C})$). What we however would like to have is the following stronger statement

$$\psi_t \xrightarrow{t\to 0} \psi_0 \qquad \text{in } L^2(\mathbb{R}^d;\mathbb{C})$$

We say then *the initial datum is continuously attained in* $L^2(\mathbb{R}^d;\mathbb{C})$ or alternatively, the map $t \mapsto \psi_t$, seen as a map from $\mathbb{R}$ to $L^2(\mathbb{R}^d;\mathbb{C})$, is continuous at $t = 0$.

Proposition 3.1.9 — The inital datum is continuously attained in L^2

Let $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ and $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution of the free Schrödinger equation with initial datum ψ_0. Then we have $\psi_t \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{t\to 0} \psi_0$.

Proof. For $t \in \mathbb{R}$ we compute

$$\|\psi_t - \psi_0\|_{L^2}^2 = \|\psi_t\|_{L^2}^2 - 2\mathrm{Re}(\langle\psi_t,\psi_0\rangle) + \|\psi_0\|_{L^2}^2 \underset{\text{Rem3.1.8}}{=\!=\!=} 2\|\psi_0\|_{L^2}^2 - 2\mathrm{Re}(\langle\psi_t,\psi_0\rangle). \tag{32}$$

Now let $\varepsilon > 0$. Choose some $\eta \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$ such that $\|\psi_0 - \eta\|_{L^2} < \varepsilon$. Now we write

$$\langle\psi_t,\psi_0\rangle = \langle\psi_t,\psi_0-\eta\rangle + \langle\psi_t,\eta\rangle. \tag{33}$$

Now note that

$$\langle\psi_t,\eta\rangle = \int_{\mathbb{R}^d} \psi_t(x)\overline{\eta(x)}\,\mathrm{d}x = L_{\psi_t}(\overline{\eta}).$$

Given that by 3.1.3 ψ_t (identified always with L_{ψ_t}) is continuous and $\overline{\eta} \in C_0^\infty(\mathbb{R};\mathbb{C})$ we have

$$\lim_{t\to 0}\langle\psi_t,\eta\rangle = \lim_{t\to 0} L_{\psi_t}(\overline{\eta}) = L_{\psi_0}(\overline{\eta}) = \int_{\mathbb{R}^d} \psi_0(x)\overline{\eta(x)}\,\mathrm{d}x = \langle\psi_0,\eta\rangle$$

For this reason we have together with (33)

$$\begin{aligned}\limsup_{t\to 0} |\langle\psi_t,\psi_0\rangle - \langle\psi_0,\eta\rangle| &\leqslant \limsup_{t\to 0} |\langle\psi_t,\psi_0-\eta\rangle| \leqslant \limsup_{t\to 0}\|\psi_t\|_{L^2}\|\psi_0-\eta\|_{L^2} \\ &\underset{\text{Rem3.1.8}}{=\!=\!=} \|\psi_0\|_{L^2}\|\psi_0-\eta\|_{L^2} \leqslant \varepsilon\|\psi_0\|_{L^2}.\end{aligned}$$

Going back to (32) we infer

$$\begin{aligned}\limsup_{t\to 0}\|\psi_t-\psi_0\|_{L^2} &\leqslant 2\|\psi_0\|_{L^2}^2 - 2\mathrm{Re}(\langle\psi_0,\eta\rangle) + 2\varepsilon\|\psi_0\|_{L^2} \\ &= 2\|\psi_0\|_{L^2}^2 - 2\mathrm{Re}(\langle\psi_0,\psi_0\rangle + \langle\psi_0,\eta-\psi_0\rangle) + 2\varepsilon\|\psi_0\|_{L^2} \\ &= 2\|\psi_0\|_{L^2}^2 - 2\|\psi_0\|^2 - 2\mathrm{Re}(\langle\psi_0,\eta-\psi_0\rangle) + 2\varepsilon\|\psi_0\|_{L^2} \\ &\leqslant 0 + 2|\langle\psi_0,\eta-\psi_0\rangle| + 2\varepsilon\|\psi_0\|_{L^2} \\ &\leqslant 2\|\psi_0\|_{L^2}\|\eta-\psi_0\|_{L^2} + 2\varepsilon\|\psi_0\|_{L^2} \leqslant 4\varepsilon\|\psi_0\|_{L^2}.\end{aligned}$$

Letting $\varepsilon \to 0$ we infer $\limsup_{t\to 0}\|\psi_t-\psi_0\|_{L^2} = 0$ and hence the claim follows.

The fact that the initial datum is even continuously attained in $L^2(\mathbb{R}^d;\mathbb{C})$ (provided that $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$) allows us to forget about the distributional background of our notion of solutions and develop the entire further theory purely in L^2.

3.1.2 The free propagator

Let $\psi_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. We have now already seen that we have a solution of the Schrödinger equation $\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$, given by Proposition 3.1.1 via

$$\psi(t,x) = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0))(x). \tag{34}$$

This solution is also unique (indeed, if there exists at most one distributional solution there can also exist at most one classical solution). We now wish to express this solution in an alternate form, which also gives rise to the precise shape of the fundamental solution, called in this case the *free propagator*.

Proposition 3.1.10 — Free Propagator — I

Let $\psi_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ and $\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ be as in Proposition 3.1.1. Then for all $t \in \mathbb{R}\backslash\{0\}$ and $x \in \mathbb{R}^d$ one has

$$\psi(t,x) = \frac{1}{(2\pi i t)^{\frac{d}{2}}}\int_{\mathbb{R}^d} e^{\frac{i|x-y|^2}{2t}}\psi_0(y)\ \mathrm{d}y. \tag{35}$$

Proof. Using (34) and the Fourier inversion formula (applicable as all the functions appearing there are Schwartz functions) we find (with $\hat{\psi}_0 := \mathcal{F}(\psi_0)$)

$$\psi(t,x) = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\psi_0))(x) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} e^{-\frac{i}{2}|p|^2 t}\hat{\psi}_0(p)e^{ip\cdot x}\ \mathrm{d}p.$$

Now note that $\hat{\psi}_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Due to this fact the absolute value of the integrand is bounded by $|\hat{\psi}_0| \in L^1$. This and the dominated convergence theorem yield

$$\begin{aligned}\int_{\mathbb{R}^d} e^{-\frac{i}{2}|p|^2 t}\hat{\psi}_0(p)e^{ip\cdot x}\ \mathrm{d}p &= \int_{\mathbb{R}^d}\lim_{\varepsilon\to 0+} e^{-\varepsilon|p|^2}e^{-\frac{i}{2}|p|^2 t}\hat{\psi}_0(p)e^{ip\cdot x}\ \mathrm{d}p \\ &= \lim_{\varepsilon\to 0+}\int_{\mathbb{R}^d} e^{-\varepsilon|p|^2}e^{-\frac{i}{2}|p|^2 t}\hat{\psi}_0(p)e^{ip\cdot x}\ \mathrm{d}p,\end{aligned}$$

i.e. (replacing $\lim\limits_{\varepsilon\to 0+}$ by $\lim\limits_{\varepsilon\to 0}$ for notational convenience)

$$\psi(t,x) = \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} e^{-\varepsilon|p|^2}e^{-\frac{i}{2}|p|^2 t}\hat{\psi}_0(p)e^{ip\cdot x}\ \mathrm{d}p = \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2}e^{ip\cdot x}\hat{\psi}_0(p)\ \mathrm{d}p.$$

Now we also know that $\hat{\psi}_0(p) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int\limits_{\mathbb{R}^d}\psi_0(y)e^{-ip\cdot y}\ \mathrm{d}y$. Our goal is to use this in the previous formula and switch the order of the two integrals appearing there by means of Fubini's theorem. Before doing so one has to ensure

$$(p,y) \mapsto e^{-(\frac{i}{2}t+\varepsilon)|p|^2}e^{ip\cdot x}\psi_0(y)e^{-ip\cdot y} \qquad \text{is integrable on } \mathbb{R}^{2d}.$$

This is readily checked since its absolute value is given by $e^{-\varepsilon|p|^2}|\psi_0(y)|$, which is integrable as product of two integrable functions that depend on distinct variables (Exercise: Use

Tonelli's Theorem).[a] Using this we find

$$
\begin{aligned}
\psi(t,x) &= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2} e^{ip\cdot x} \hat{\psi}_0(p)\,\mathrm{d}p \\
&= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d}} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2} e^{ip\cdot x} \psi_0(y) e^{-ip\cdot y}\,\mathrm{d}y\,\mathrm{d}p \\
&= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d}} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2} e^{ip\cdot x} \psi_0(y) e^{-ip\cdot y}\,\mathrm{d}p\,\mathrm{d}y \\
&= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d}} \int_{\mathbb{R}^d} \psi_0(y) \int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2} e^{-ip\cdot(y-x)}\,\mathrm{d}p\,\mathrm{d}y. \qquad (36)
\end{aligned}
$$

Now since for any $\varepsilon > 0$ the map $p \mapsto e^{(-\frac{i}{2}t+\varepsilon)|p|^2}$ lies in $\mathcal{S}(\mathbb{R}^d;\mathbb{C})$ we obtain

$$
\int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2} e^{-ip\cdot(y-x)}\,\mathrm{d}p = (2\pi)^{\frac{d}{2}} \mathcal{F}(e^{-(\frac{i}{2}t+\varepsilon)|\cdot|^2})(y-x).
$$

Using that for any $\alpha \in \mathbb{C}$ with $\mathrm{Re}(\alpha) > 0$ we have $\mathcal{F}(e^{-|\cdot|^2\alpha}) = (2\alpha)^{-\frac{d}{2}} e^{-\frac{|\cdot|^2}{4\alpha}}$ (Exercise, cf. also Step 1 in Proof of Theorem 4.5) we obtain (with $\alpha = \frac{i}{2}t + \varepsilon$, $\varepsilon > 0$) that

$$
\int_{\mathbb{R}^d} e^{-(\frac{i}{2}t+\varepsilon)|p|^2} e^{-ip\cdot(y-x)}\,\mathrm{d}p = (2\pi)^{\frac{d}{2}} \frac{1}{(it+2\varepsilon)^{\frac{d}{2}}} e^{-\frac{|y-x|^2}{2it+4\varepsilon}}.
$$

Using this in (36) we obtain

$$
\psi(t,x) = \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{\frac{d}{2}}} \frac{1}{(it+2\varepsilon)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \psi_0(y) e^{-\frac{|y-x|^2}{2it+4\varepsilon}}\,\mathrm{d}y. \qquad (37)
$$

Now we need to let $\varepsilon \to 0$ inside the integral. It is clear that the pointwise limit of the integrand is given by $y \mapsto \psi_0(y) e^{-\frac{|y-x|^2}{2it}} = \psi_0(y) e^{i\frac{|x-y|^2}{2t}}$. To find an integrable dominating function we estimate for $y \in \mathbb{R}^d$ and $\varepsilon > 0$

$$
\begin{aligned}
|\psi_0(y) e^{-\frac{|y-x|^2}{2it+4\varepsilon}}| &= |\psi_0(y)| e^{-\mathrm{Re}(\frac{|y-x|^2}{2it+4\varepsilon})} \\
&= |\psi_0(y)| e^{-\mathrm{Re}(\frac{|y-x|^2}{4t^2+16\varepsilon^2}(4\varepsilon-2it))} = |\psi_0(y)| e^{\frac{-4\varepsilon|y-x|^2}{4t^2+16\varepsilon^2}} \leqslant |\psi_0(y)|.
\end{aligned}
$$

This now allows us to pass to the limit inside the integral in (37) and obtain

$$
\psi(t,x) = \frac{1}{(2\pi)^{\frac{d}{2}}} \frac{1}{(it)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \psi_0(y) e^{-\frac{|x-y|^2}{2it}}\,\mathrm{d}y = \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \psi_0(y) e^{i\frac{|x-y|^2}{2t}}\,\mathrm{d}y.
$$

The claim follows.

[a] Observe that this is the reason why we introduced the parameter ε at all: For $\varepsilon = 0$ the resulting expression is not integrable with respect to p.

The function that appears in (35) can be seen as a sort of *fundamental solution* of the free Schrödinger equation (cf. Lecture 9 in Part II). Such a fundamental solution must exist by the Malgrange Ehrenpreis Theorem (Theorem 9.2 in Part II).

Definition 3.1.11 — FREE PROPAGATOR

The function $P_0 : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ given by

$$P_0(t; x, y) := \frac{1}{(2\pi i t)^{\frac{d}{2}}} e^{i\frac{|x-y|^2}{2t}}$$

is called the *free propagator*.

The solution formula (35) holds so far only true for initial data in $\mathcal{S}(\mathbb{R}^d; \mathbb{C})$. As always we would like to treat more irregular initial data in $L^2(\mathbb{R}^d; \mathbb{C})$. This can easily be studied by means of Proposition 3.1.7. Indeed: Fix $\psi_0 \in L^2(\mathbb{R}^d; \mathbb{C})$ arbitrary and let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d; \mathbb{C})$ be the unique distributional solution to the Schrödinger equation with initial value ψ_0. Choose $(\psi_0^{(n)})_{n\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ such that $\psi_0^{(n)} \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_0$. Now, if $\psi^{(n)} : \mathbb{R} \to L^2(\mathbb{R}^d; \mathbb{C})$ is the unique distributional solution with initial datum $\psi_0^{(n)}$ we have by Proposition 3.1.10 for any $t \in \mathbb{R}\backslash\{0\}$

$$\forall x \in \mathbb{R}^d : \qquad \psi_t^{(n)}(x) = \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}} e^{\frac{i|x-y|^2}{2t}} \psi_0^{(n)}(y)\, \mathrm{d}y. \tag{38}$$

Moreover, we know that

$$\|\psi_t^{(n)} - \psi_t\|_{L^2} = \|\psi_0^{(n)} - \psi_0\|_{L^2} \xrightarrow{n\to\infty} 0,$$

that is $\psi_t^{(n)} \xrightarrow[L^2(\mathbb{R}^d,\mathbb{C})]{n\to\infty} \psi_t$. Summarized we can proceed for given $\psi_0 \in L^2(\mathbb{R}^d; \mathbb{C})$ as follows

- Choose $(\psi_0^{(n)})_{n\in\mathbb{N}} \subseteq \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ such that $\psi_0^{(n)} \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} \psi_0$
- Form for $t \in \mathbb{R}\backslash\{0\}$ the expression on the right hand side of (38) and interpret it as a function of $x \in \mathbb{R}^d$
- Figure out its L^2-limit $\underset{n\to\infty}{\mathrm{LIM}}\ \psi_t^{(n)}$. This is then ψ_t, the solution at time t with inital value ψ_0.

Remark 3.1.12 — LACK OF REPRESENTATION FORMULA

Unfortunately ψ_t can for general $\psi_0 \in L^2(\mathbb{R}^d; \mathbb{C})$ not be expressed in such a nice formula as in (35). This is readily checked: Suppose that $\psi_0 \in L^2(\mathbb{R}^d; \mathbb{C})\backslash L^1(\mathbb{R}^d; \mathbb{C})$ (e.g. one could choose $\psi_0(x) = \frac{1}{1+|x|^\alpha}$ for some $\alpha \in (\frac{d}{2}, d])$. Then the expression on the right hand side of (35) is not well-defined, since

$$y \mapsto \left| e^{i\frac{|x-y|^2}{2t}} \psi_0(y) \right| = |\psi_0(y)|,$$

is not integrable for any $x \in \mathbb{R}^d$. Hence the above approximation procedure will not end up in a nice formula.

With one further mild regularity on ψ_0, a solution formula can however be obtained and carries over from 3.1.10.

Theorem 3.1.13 — The Free Propagator — II

Suppose that $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$. Let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution of the free Schrödinger equation with initial datum ψ_0. Then for each $t \in \mathbb{R}\backslash\{0\}$ there holds

$$\psi_t(x) = \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y \qquad \text{for a.e. } x \in \mathbb{R}^d.$$

From the next proof onwards we will denote for a set $A \subset \mathbb{R}^d$ the *characteristic function* $\chi_A : \mathbb{R}^d \to \mathbb{R}$ to be given by

$$\chi_A(x) := \begin{cases} 1 & x \in A \\ 0 & x \notin A \end{cases}.$$

Proof of Theorem 3.1.13. Let $\psi_0 \in L^1(\mathbb{R}^d;\mathbb{C}) \cap L^2(\mathbb{R}^d;\mathbb{C})$ be as in the statement and let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C}), t \mapsto \psi_t$ be the unique distributional solution of the Schrödinger equation with initial datum ψ_0. We start with the following

Intermediate claim. There exists $(\psi_0^{(n)})_{n\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ such that $\psi_0^{(n)} \xrightarrow[L^1(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_0$ and $\psi_0^{(n)} \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_0$.

We leave the details here as an exercise. Just a rough sketch: One readily checks that $\psi_0\chi_{B_n(0)} \xrightarrow[L^1(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_0$ and $\psi_0\chi_{B_n(0)} \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \psi_0$. Let next $(\varphi_\varepsilon)_{\varepsilon>0} \subseteq C_0^\infty(\mathbb{R}^d;\mathbb{C})$ be an approximation to the identity in the sense of Part I Definition 1.3.9. Now, for each $\varepsilon > 0$ one has that $\psi_0\chi_{B_n(0)} * \varphi_\varepsilon$ lies in $C_0^\infty(\mathbb{R}^d;\mathbb{C}) \subset \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Moreover, as $\varepsilon \to 0$ we have the convergences $\psi_0\chi_{B_n(0)} * \varphi_\varepsilon \xrightarrow[L^1(\mathbb{R}^d;\mathbb{C})]{\varepsilon\to 0} \psi_0\chi_{B_n(0)}$ and $\psi_0\chi_{B_n(0)} * \varphi_\varepsilon \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{\varepsilon\to 0} \psi_0\chi_{B_n(0)}$ (these can be obtained in a similar way as in exercise sheet 1 of part III, exercise 4). In particular we can choose $\varepsilon_n > 0$ such that

$$\|\psi_0\chi_{B_n(0)} * \varphi_{\varepsilon_n} - \psi_0\chi_{B_n(0)}\|_{L^1} + \|\psi_0\chi_{B_n(0)} * \varphi_{\varepsilon_n} - \psi_0\chi_{B_n(0)}\|_{L^2} < \frac{1}{n}.$$

If we now choose $\psi_0^{(n)} := \psi_0\chi_{B_n(0)} * \varphi_{\varepsilon_n}$ we have

$$\|\psi_0^{(n)} - \psi_0\|_{L^1} \leqslant \|\psi_0^{(n)} - \psi_0\chi_{B_n(0)}\|_{L^1} + \|\psi_0\chi_{B_n(0)} - \psi_0\|_{L^1} \leqslant \frac{1}{n} + \|\psi_0\chi_{B_n(0)} - \psi_0\|_{L^1} \xrightarrow{n\to\infty} 0$$

and

$$\|\psi_0^{(n)}-\psi_0\|_{L^2}\leqslant\|\psi_0^{(n)}-\psi_0\chi_{B_n(0)}\|_{L^2}+\|\psi_0\chi_{B_n(0)}-\psi_0\|_{L^2}\leqslant\frac{1}{n}+\|\psi_0\chi_{B_n(0)}-\psi_0\|_{L^2}\xrightarrow{n\to\infty}0.$$

The intermediate claim follows.

Let $(\psi_0^{(n)})_{n\in\mathbb{N}}$ be as in the intermediate claim. The unique distributional solution $\psi^{(n)}$ of the Schrödinger equation satisfies for $t\in\mathbb{R}\backslash\{0\}$ and $x\in\mathbb{R}^d$

$$\psi_t^{(n)}(x)=\frac{1}{(2\pi it)^{\frac{d}{2}}}\int_{\mathbb{R}^d}e^{i\frac{|x-y|^2}{2t}}\psi_0^{(n)}(y)\,\mathrm{d}y.$$

We now determine pointwise limits of the right hand side and (up to a subsequence) of the left hand side. Let us first treat the right hand side. For $x\in\mathbb{R}^d$ and $t\in\mathbb{R}\backslash\{0\}$ we have

$$\begin{aligned}&\left|\frac{1}{(2\pi it)^{\frac{d}{2}}}\int_{\mathbb{R}^d}e^{i\frac{|x-y|^2}{2t}}\psi_0^{(n)}(y)\,\mathrm{d}y-\frac{1}{(2\pi it)^{\frac{d}{2}}}\int_{\mathbb{R}^d}e^{i\frac{|x-y|^2}{2t}}\psi_0(y)\,\mathrm{d}y\right|\\&=\frac{1}{(2\pi|t|)^{\frac{d}{2}}}\left|\int_{\mathbb{R}^d}e^{i\frac{|x-y|^2}{2t}}(\psi_0^{(n)}(y)-\psi_0(y))\,\mathrm{d}y\right|\leqslant\frac{1}{(2\pi|t|)^{\frac{d}{2}}}\int_{\mathbb{R}^d}|e^{i\frac{|x-y|^2}{2t}}|\,|\psi_0^{(n)}(y)-\psi_0(y)|\,\mathrm{d}y\\&=\frac{1}{(2\pi|t|)^{\frac{d}{2}}}\int_{\mathbb{R}^d}|\psi_0^{(n)}(y)-\psi_0(y)|\,\mathrm{d}y=\frac{1}{(2\pi|t|)^{\frac{d}{2}}}\|\psi_0^{(n)}-\psi_0\|_{L^1}\xrightarrow{n\to\infty}0.\end{aligned}$$

Hence the right hand side converges pointwise to

$$x\mapsto\frac{1}{(2\pi it)^{\frac{d}{2}}}\int_{\mathbb{R}^d}e^{i\frac{|x-y|^2}{2t}}\psi_0(y)\,\mathrm{d}y.\tag{39}$$

Now we look at the left hand side. First observe that by Proposition 3.1.7 we have

$$\|\psi_t^{(n)}-\psi_t\|_{L^2}=\|\psi_0^{(n)}-\psi_0\|_{L^2}\xrightarrow{n\to\infty}0,$$

that is $\psi_t^{(n)}\xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty}\psi_t$. By Proposition 2.3.17 in Analysis III there exists a subsequence $(\ell_n)_{n\in\mathbb{N}}\subset\mathbb{N}$ such that $(\psi_t^{(\ell_n)})_{n\in\mathbb{N}}$ converges pointwise a.e. to ψ_t, i.e. for a.e. $x\in\mathbb{R}^d$ we have $\lim\limits_{n\to\infty}\psi_t^{(\ell_n)}(x)=\psi_t(x)$. However, for all such $x\in\mathbb{R}^d$ the limit $\lim\limits_{n\to\infty}\psi_t^{(\ell_n)}(x)$ must also equal the expression in (39) (as we discussed before (39) and since subsequences of convergent sequences are convergent). Uniqueness of limits in $\mathbb{C}$ yields that for a.e. $x\in\mathbb{R}^d$ we have

$$\psi_t(x)=\frac{1}{(2\pi it)^{\frac{d}{2}}}\int_{\mathbb{R}^d}e^{i\frac{|x-y|^2}{2t}}\psi_0(y)\,\mathrm{d}y.$$

From this theorem we can indeed obtain an integral representation, just with a slightly different notion of integral

Corollary 3.1.14

Suppose that $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. Let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution of the Schrödinger equation with initial datum ψ_0. Then for each $t \in \mathbb{R}\backslash\{0\}$ we have

$$\psi_t = \operatorname*{LIM}_{m\to\infty} \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{B_m(0)} e^{i\frac{|(\cdot)-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y$$

where $\operatorname*{LIM}_{m\to\infty}$ is to be understood as L^2-limit of functions in $L^2(\mathbb{R}^d;\mathbb{C})$

Proof. Let $m \in \mathbb{N}$. Define $\psi_0^{(m)} := \chi_{B_m(0)}\psi_0$. Then $\psi_0^{(m)} \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$ as

$$\begin{aligned}\int_{\mathbb{R}^d} |\psi_0^{(m)}(y)|\, \mathrm{d}y &= \int_{B_m(0)} |\psi_0(y)|\, \mathrm{d}y \leqslant \sqrt{\int_{B_m(0)} 1\, \mathrm{d}y}\sqrt{\int_{B_m(0)} |\psi_0(y)|^2\, \mathrm{d}y} \\ &= \sqrt{|B_m(0)|}\sqrt{\int_{B_m(0)} |\psi_0(y)|^2\, \mathrm{d}y} \leqslant \sqrt{|B_m(0)|}\sqrt{\int_{\mathbb{R}^d} |\psi_0(y)|^2\, \mathrm{d}y} < \infty.\end{aligned}$$

In particular, Theorem 3.1.13 implies that if $\psi^{(m)} : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ is the unique distributional solution to the free Schrödinger equation with initial datum $\psi_0^{(m)}$ we have

$$\psi_t^{(m)}(x) = \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0^{(m)}(y)\, \mathrm{d}y = \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{B_m(0)} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y. \tag{40}$$

Now we have

$$\|\psi_0 - \psi_0^{(m)}\|_{L^2}^2 = \int_{\mathbb{R}^d} |\psi_0(x) - \psi_0(x)\chi_{B_m(0)}(x)|^2\, \mathrm{d}x = \int_{\mathbb{R}^d} |\psi_0(x)|^2\, |1 - \chi_{B_m(0)}(x)|^2\, \mathrm{d}x \xrightarrow{m\to\infty} 0,$$

by the dominated convergence theorem (due to the fact that $1 - \chi_{B_m(0)} \xrightarrow[ptw]{m\to\infty} 0$ and the fact that for all $m \in \mathbb{N}$ we have $|\psi_0|^2|1-\chi_{B_m(0)}|^2 \leqslant |\psi_0|^2$, which is integrable). Now, Proposition 3.1.7 yields

$$\|\psi_t - \psi_t^{(m)}\|_{L^2} = \|\psi_0 - \psi_0^{(m)}\|_{L^2}^2 \xrightarrow{m\to\infty} 0$$

so that by

$$\psi_t = \operatorname*{LIM}_{m\to\infty} \psi_t^{(m)} \underset{(40)}{=} \operatorname*{LIM}_{m\to\infty} \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{B_m(0)} e^{i\frac{|(\cdot)-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y$$

For later use we will actually give this expression a name: For $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ we define (for a.e. $x \in \mathbb{R}^d$)

$$\tilde{\int}_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y := \left[\operatorname*{LIM}_{m\to\infty} \int_{B_m(0)} e^{i\frac{|(\cdot)-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y\right](x), \tag{41}$$

i.e. we take the L^2-limit of the expression inside the brackets (which exists due to the previous corollary) and evaluate it at x. This notatin will later be of use, when we talk about path integrals.

3.1.3 Long time behavior

Now we have a formula for solutions of the Schrödinger equation in $L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$. We should now be interested in consequences of this formula. What can one really learn about solutions if one has the representation with the free propagator? One thing that seems very accessible now is *long-time behavior*, i.e. what happens to solutions as $t \to \infty$. The following is a relatively immediate consequence of Theorem 3.1.13.

Proposition 3.1.15 — Asymptotic behavior — I

Let $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$ and let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique solution with initial datum ψ_0. Then

$$\lim_{t\to\infty} \|\psi_t\|_{L^\infty} = 0.$$

Proof. Let $t > 0$. And $N_t \subset \mathbb{R}^d$ be a Lebesgue null set such that

$$\psi_t(x) = \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y \qquad \text{for all } x \in \mathbb{R}^d \backslash N_t.$$

(Note that such set N_t exists due to Theorem 3.1.13). Then for $x \in \mathbb{R}^d\backslash N_t$ we have

$$\begin{aligned} |\psi_t(x)| &= \frac{1}{(2\pi t)^{\frac{d}{2}}} \left| \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\, \mathrm{d}y \right| \\ &\leqslant \frac{1}{(2\pi t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \left| e^{i\frac{|x-y|^2}{2t}} \psi_0(y) \right| \mathrm{d}y = \frac{1}{(2\pi t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} |\psi_0(y)|\, \mathrm{d}y. \end{aligned}$$

This implies according to Proposition 2.3.2 in ↑ `Analysis III Lecture Notes`

$$\|\psi_t\|_{L^\infty} \leqslant \sup_{x\in\mathbb{R}^d\backslash N_t} |\psi_t(x)| \leqslant \frac{1}{(2\pi t)^{\frac{d}{2}}} \|\psi_0\|_{L^1} \xrightarrow{t\to\infty} 0.$$

This means in a certain sense that for $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$ $t \mapsto \psi_t$ must *spread out*. Indeed, the fact that $t \mapsto \|\psi_t\|_{L^\infty}$ is small means that ψ_t can only attain small values. The fact that however $t \mapsto \|\psi_t\|_{L^2} = \|\psi_0\|_{L^2}$ is bounded below (unless $\psi_0 \neq 0$) means that these small values must be attained on a larger set, to ensure that the L^2-norm is constant.
We will now formulate with more mathematical precision what this spreading out means. To this end we recall that for a function $f \in L^1_{\mathrm{loc}}(R^d;\mathbb{C})$ we say that a point x_0 lies in the *non-support* of f if there exists $r > 0$ such that $f|_{B_r(x_0)} = 0$ Lebesgue almost everywhere. The set of all points in the non-support of f is denoted by $\mathrm{spt}(f)^C$ and its complement is denoted $\mathrm{spt}(f)$ and called *support* of f. This notion is consistend with Definition 1.3.12 of

part I in the sense that $\text{spt}(f) = \text{supp}(L_f)$. Note that for a set $K \subset \mathbb{R}^d$ compact we have the following statement

$$\text{spt}(f) \subseteq K \qquad \Longleftrightarrow \qquad f|_{\mathbb{R}^d \setminus K} = 0 \text{ Lebesgue a.e.}$$

We will now show that solution spread out in the sense that

Proposition 3.1.16

Suppose that $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ be such that there exists $K \subset \mathbb{R}^d$ such that $\text{spt}(\psi_0) \subseteq K$. Let $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution to the Schrödinger equation. Then either $\psi_0 = 0$ a.e. or for each compact set $K' \subset \mathbb{R}^d$ one can find a time $t' > 0$ such that $\text{spt}(\psi_{t'}) \cap (K')^C \neq \varnothing$.

Proof. Before we start with the proof notice that actually $\psi_0 \in L^1(\mathbb{R}^d;\mathbb{C}) \cap L^2(\mathbb{R}^d;\mathbb{C})$ (i.e. ψ does not just lie in L^2 but also in L^1). Indeed, the Cauchy-Schwarz inequality yields

$$\int_{\mathbb{R}^d} |\psi_0(y)| \, \mathrm{d}y = \int_K |\psi_0(y)| \, \mathrm{d}y \leqslant \sqrt{\int_K |\psi_0(y)|^2 \, \mathrm{d}y} \sqrt{\lambda_d(K)} \leqslant \sqrt{\lambda_d(K)} \|\psi_0\|_{L^2} < \infty.$$

Now let's begin with the proof. Suppose that $\text{spt}(\psi_t) \subset K'$ for all $t > 0$. Then for all $t > 0$ we have

$$\begin{aligned} \|\psi_0\|_{L^2}^2 = \|\psi_t\|_{L^2}^2 &= \int_{\mathbb{R}^d} |\psi_t(x)|^2 \, \mathrm{d}x \\ &= \int_{K'} |\psi_t(x)|^2 \, \mathrm{d}x \leqslant \int_{K'} \|\psi_t\|_{L^\infty}^2 \, \mathrm{d}x = \|\psi_t\|_{L^\infty}^2 \lambda_d(K') \xrightarrow{t\to\infty} 0, \end{aligned}$$

where we used 3.1.15 in the last step. This yields $\|\psi_0\|_{L^2} = 0$ and thus $\psi_0 = 0$ a.e. In particular, if "$\psi_0 = 0$ a.e." is not true then there must exist $t' > 0$ such that $\text{spt}(\psi_t) \nsubseteq K'$. The claim follows.

So far we had the restriction that the inital datum lies in $L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$. We would like to find asymptotics that hold for general intial data in $L^2(\mathbb{R}^d;\mathbb{C})$

Proposition 3.1.17

Let $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. For $t \in \mathbb{R}\setminus\{0\}$ define $L_t : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ via

$$L_t(\psi_0)(x) := \frac{1}{(it)^{\frac{d}{2}}} e^{i\frac{|x|^2}{2t}} \mathcal{F}(\psi_0)(\tfrac{x}{t}) \qquad \text{a.e. } x \in \mathbb{R}^d$$

Then the unique distributional solution $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ with initial value ψ_0 satisfies

$$\lim_{t\to\infty} \|\psi_t - L_t(\psi_0)\|_{L^2} = 0.$$

Proof. We first show this in the special case of $\psi_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. In this case we have for $x \in \mathbb{R}^d$

$$\begin{aligned}
\psi_t(x) - L_t(\psi_0)(x) &= \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\,\mathrm{d}y - \frac{1}{(it)^{\frac{d}{2}}} e^{i\frac{|x|^2}{2t}} \mathcal{F}(\psi_0)(\tfrac{x}{t}) \\
&= \frac{1}{(2\pi i t)^{\frac{d}{2}}} \left(\int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y)\,\mathrm{d}y - e^{i\frac{|x|^2}{2t}} \int_{\mathbb{R}^d} \psi_0(y) e^{-iy\cdot\frac{x}{t}}\,\mathrm{d}y \right) \\
&= \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \psi_0(y) \left(e^{i\frac{|x-y|^2}{2t}} - e^{i(\frac{|x|^2}{2t} - \frac{x\cdot y}{t})} \right) \mathrm{d}y \\
&= \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \psi_0(y) \left(e^{i\frac{|x|^2 - 2x\cdot y + |y|^2}{2t}} - e^{i(\frac{|x|^2}{2t} - \frac{x\cdot y}{t})} \right) \mathrm{d}y \\
&= \frac{1}{(2\pi i t)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \psi_0(y) e^{i\frac{|x|^2}{2t}} e^{-i\frac{x\cdot y}{t}} \left(e^{i\frac{|y|^2}{2t}} - 1 \right) \mathrm{d}y \\
&= \frac{1}{(it)^{\frac{d}{2}}} e^{i\frac{|x|^2}{2t}} \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}} \psi_0(y) \left(e^{i\frac{|y|^2}{2t}} - 1 \right) e^{-iy\cdot\frac{x}{t}}\,\mathrm{d}y = \frac{1}{(it)^{\frac{d}{2}}} e^{i\frac{|x|^2}{2t}} \mathcal{F}(g_t)(\tfrac{x}{t}),
\end{aligned}$$

where $g_t \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ is given by $g_t(y) := \psi_0(y)\left(e^{i\frac{|y|^2}{2t}} - 1\right)$ ([a]). We infer that

$$\|\psi_t - L_t(\psi_0)\|_{L^2}^2 = \int_{\mathbb{R}^d} |\psi_t(x) - L_t(\psi_0)(x)|^2\,\mathrm{d}x = \tfrac{1}{t^d} \int_{\mathbb{R}^d} |\mathcal{F}(g_t)(\tfrac{x}{t})|^2\,\mathrm{d}x$$

Using the transformation $\Phi : \mathbb{R}^d \to \mathbb{R}^d, x \mapsto \frac{x}{t}$ and obeserving that $\det(D\Phi(x)) = \det(\frac{1}{t}\mathrm{Id}) = \frac{1}{t^d}$ we find

$$\|\psi_t - L_t(\psi_0)\|_{L^2}^2 = \int_{\mathbb{R}^d} |\mathcal{F}(g_t)(p)|^2\,\mathrm{d}p = \int_{\mathbb{R}^d} |g_t(x)|^2\,\mathrm{d}x = \int_{\mathbb{R}^d} |\psi_0(x)|^2 \left|e^{i\frac{|x|^2}{2t}} - 1\right|^2 \mathrm{d}q.$$

One readily checks that as $t \to \infty$ the integrand converges to 0 pointwise. Moreover $\left|e^{i\frac{|x|^2}{2t}} - 1\right| \leqslant |e^{i\frac{|x|^2}{2t}}| + |1| = 2$, which is why the integrand is bounded above by $x \mapsto 4|\psi_0(x)|^2$, which is integrable on $\mathbb{R}^d$ as $\psi_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. We obtain therefore

$$\lim_{t\to\infty} \|\psi_t - L_t(\psi_0)\|_{L^2}^2 = 0.$$

Next we study general initial data $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. Let $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$ and $\varepsilon > 0$ be arbitrary. An approximation result (cf. Sheet 1 Exercise 4 of part III) implies that there exists $\tilde{\psi}_0 \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$ with the property that $\|\psi_0 - \tilde{\psi}_0\|_{L^2} < \varepsilon$. Note in particular that $\tilde{\psi}_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Let $\tilde{\psi} : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ be the unique distributional solution to the Schrödinger equation with initial datum $\tilde{\psi}_0$. Then, according to Proposition 3.1.7

$$\|\tilde{\psi}_t - \psi_t\|_{L^2} = \|\tilde{\psi}_0 - \psi_0\|_{L^2} < \varepsilon.$$

Moreover,

$$\begin{aligned} \|L_t(\tilde{\psi}_0) - L_t(\psi_0)\|_{L^2}^2 &= \|L_t(\tilde{\psi}_0 - \psi_0)\|_{L^2}^2 = \tfrac{1}{t^d} \int_{\mathbb{R}^d} |\mathcal{F}(\tilde{\psi}_0 - \psi_0)(\tfrac{x}{t})|^2 \,\mathrm{d}x \\ &= \int_{\mathbb{R}^d} |\mathcal{F}(\tilde{\psi}_0 - \psi_0)(y)|^2 \,\mathrm{d}y = \|\mathcal{F}(\tilde{\psi}_0 - \psi_0)\|_{L^2}^2 = \|\tilde{\psi}_0 - \psi_0\|_{L^2}^2 < \varepsilon^2, \end{aligned}$$

so that

$$\|L_t(\tilde{\psi}_0) - L_t(\psi_0)\|_{L^2} < \varepsilon.$$

Hence we have

$$\begin{aligned} \|\psi_t - L_t(\psi_0)\|_{L^2} &= \|\psi_t - \tilde{\psi}_t + \tilde{\psi}_t - L_t(\tilde{\psi}_0) + L_t(\tilde{\psi}_0) - L_t(\psi_0)\|_{L^2} \\ &\leqslant \|\psi_t - \tilde{\psi}_t\| + \|\tilde{\psi}_t - L_t(\tilde{\psi}_0)\|_{L^2} + \|L_t(\tilde{\psi}_0) - L_t(\psi_0)\|_{L^2} \\ &\leqslant \varepsilon + \|\tilde{\psi}_t - L_t(\tilde{\psi}_0)\|_{L^2} + \varepsilon. \end{aligned}$$

Due to the fact that we have already shown the claim for Schwartz functions we have $\lim_{t\to\infty}\|\tilde{\psi}_t - L_t(\tilde{\psi}_0)\|_{L^2} = 0$. Using this in te previous chain of inequalities yields

$$\limsup_{t\to\infty}\|\psi_t - L_t(\psi_0)\|_{L^2} \leqslant 2\varepsilon.$$

Since $\varepsilon > 0$ was arbitary, we conclude

$$\limsup_{t\to\infty}\|\psi_t - L_t(\psi_0)\|_{L^2} = 0,$$

and hence also $\lim\limits_{t\to\infty}\|\psi_t - L_t(\psi_0)\|_{L^2} = 0$.

[a]At this point one would actually have to check that the function g defined by the formula above actually lies in $\mathcal{S}(\mathbb{R}^d;\mathbb{C})$. We leave this as an exercise.

3.2 Schrödinger equation with potentials

We have now understood the Schrödinger equation without potential. However, most interesting physical systems do have a potential and therefore satisfy (15) with $V \not\equiv 0$. However, if $V \not\equiv 0$ we have not even understood how to read (15) (since again L^2-functions do not necessarily have a derivative)! Since V is not constant, Fourier analysis techniques are not immediately applicable, so the apporoach of the previous section can not be pursued. We have to change our point of view.
Fix again $\psi_0 \in L^2(\mathbb{R}^d;\mathbb{C})$. Instead of describing the solution $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C})$ at a time t we seek to describe the *evolution operator* $U(t) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$, which is the operator

that safisfies

$$U(t)(\psi_0) = \psi(t, \cdot).$$

Why is that easier than describing ψ? Let us be inspired by the case $V \equiv 0$.
In this case, Remark 3.1.8 suggests that $U(t) : L^2(\mathbb{R}^d; \mathbb{C}) \to L^2(\mathbb{R}^d; \mathbb{C})$ is a bounded linear operator defined on the whole of $L^2(\mathbb{R}^d; \mathbb{C})$. Even more, it is also an *isometry* of $L^2(\mathbb{R}^d; \mathbb{C})$! Therefore, the operator $U(t)$ is much easier to handle than operators involving derivatives, which are not defined on the whole of $L^2(\mathbb{R}^d; \mathbb{C})$. This is why we now focus on the description the operator family $(U(t))_{t\in\mathbb{R}}$ instead of the symbols in (15). We first seek to characterize the family $(U(t))_{t\in\mathbb{R}}$ by its fundamental properties.

Definition 3.2.1 — Unitary one-parameter groups

A family $(U(t))_{t\in\mathbb{R}}$ of linear operators from $L^2(\mathbb{R}^d; \mathbb{C})$ to $L^2(\mathbb{R}^d; \mathbb{C})$ is called a *stongly continuous unitary one-parameter group* (short: SCU-group) if the following holds

(U1) *Isometry.* For all $t \in \mathbb{R}$ we have $\|U(t)\varphi\|_{L^2} = \|\varphi\|_{L^2}$ for all $\varphi \in L^2(\mathbb{R}^d; \mathbb{C})$

(U2) *Strong continuity.* We have $\lim_{t\to 0}\|U(t)\varphi - \varphi\|_{L^2} = 0$ for all $\varphi \in L^2(\mathbb{R}^d; \mathbb{C})$

(U3) *Group Property.* We have $U(0) = \mathrm{id}$ and for all $t, s \in \mathbb{R}$ we have $U(t+s) = U(t)\circ U(s)$. We also leave out the $\circ$ for the sake of notational simplicity and write $U(t + s) = U(t)U(s)$.

We will justify the Axioms (U1),(U2),(U3) by showing that they are satisfied by the free propagator in the special case of $V = 0$.

Example 3.2.2

Let $t \in \mathbb{R}$. We define a linear operator $U(t) : L^2(\mathbb{R}^d; \mathbb{C}) \to L^2(\mathbb{R}^d; \mathbb{C})$ as follows. For $\varphi \in L^2(\mathbb{R}^d; \mathbb{C})$ we set

$$U(t)\varphi := (\psi_\varphi)_t$$

where $\psi_\varphi : \mathbb{R} \to L^2(\mathbb{R}^d; \mathbb{C}), t \mapsto (\psi_\varphi)_t$ is the unique distributional solution to the free Schrödinger equation with initial datum φ. We also recall from Theorem 3.1.4 that $U(t)\varphi = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\varphi))$ for all $t \in \mathbb{R}$.

Claim. $(U(t))_{t\in\mathbb{R}}$ defines an SCU-group.

We leave it as an exercise to check that $U(t)$ is a linear operator from $L^2(\mathbb{R}^d; \mathbb{C})$ to itself. Now we check all the three axioms.

Proof of (U1). Thanks to Remark 3.1.8 we have for each $t \in \mathbb{R}$

$$\|U(t)\varphi\|_{L^2} = \|(\psi_\varphi)_t\|_{L^2} = \|(\psi_\varphi)_0\|_{L^2} = \|\varphi\|_{L^2}.$$

The claim follows.

Proof of (U2). Thanks to Proposition 3.1.9 we have

$$\lim_{t\to 0}\|U(t)\varphi - \varphi\|_{L^2} = \lim_{t\to 0}\|(\psi_\varphi)_t - \varphi\|_{L^2} = \lim_{t\to 0}\|(\psi_\varphi)_t - (\psi_\varphi)_0\|_{L^2} = 0.$$

Proof of (U3). For $t = 0$ we have

$$U(0)\varphi = (\psi_\varphi)_0 = \varphi \qquad \forall \varphi \in L^2(\mathbb{R}^d;\mathbb{C})$$

It remains to show that for $t, s \in \mathbb{R}$ we have $U(t+s) = U(t)\circ U(s)$. To this end let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. Then

$$U(t+s)\varphi = (\psi_\varphi)_{t+s}$$

One readily checks with definition 3.1.2 that $t \mapsto (\psi_\varphi)_{t+s}$ is a distributional solution of the free Schrödinger equation. As a result it is the unique distributional solution of the free Schrödinger equation with initial datum $(\psi_\varphi)_{0+s} = (\psi_\varphi)_s = U(s)\varphi$. As a result $t \mapsto U(t+s)\varphi$ is the unique distributional solution of the free Schrödinger equation with initial datum $U(s)\varphi$ and hence coincides with $t \mapsto U(t)(U(s)\varphi) = (U(t)\circ U(s))\varphi$.

There are some other helpful consequences of (U1),(U2),(U3)

Remark 3.2.3 — Invertibility

Let $(U(t))_{t\in\mathbb{R}}$ be an SCU-group. We claim that for all $t \in \mathbb{R}$ the map $U(t) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is invertible in $L^2(\mathbb{R}^d;\mathbb{C})$ and $U(t)^{-1} = U(-t)$.

This is readily checked with (U3). One has

$$U(t)\circ U(-t) = U(t + (-t)) = U(0) = \mathrm{id}.$$

and similarly also

$$U(-t)\circ U(t) = U(-t+t) = U(0) = \mathrm{id}.$$

Remark 3.2.4 — Unitariness

While the word "unitary" appears in the name of an SCU-group it is not clear from the axioms that for each $t \in \mathbb{R}$ the operator $U(t) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is *unitary*, i.e. for each $\varphi_1, \varphi_2 \in L^2(\mathbb{R}^d;\mathbb{C})$ we have

$$\langle U(t)\varphi_1, U(t)\varphi_2\rangle = \langle \varphi_1, \varphi_2\rangle \tag{42}$$

Proof of (42)**.** This is similar to the proof of the intermediate claim in Proposition 2.2.12.

First we compute

$$\begin{aligned}\|\varphi_1+\varphi_2\|_{L^2}^2-\|\varphi_1\|_{L^2}^2-\|\varphi_2\|_{L^2}^2 &= \langle\varphi_1+\varphi_2,\varphi_1+\varphi_2\rangle-\langle\varphi_1,\varphi_1\rangle-\langle\varphi_2,\varphi_2\rangle\\ &= \langle\varphi_1,\varphi_1\rangle+\langle\varphi_1,\varphi_2\rangle+\langle\varphi_2,\varphi_1\rangle+\langle\varphi_2,\varphi_2\rangle-\langle\varphi_1,\varphi_1\rangle-\langle\varphi_2,\varphi_2\rangle\\ &= \langle\varphi_1,\varphi_2\rangle+\langle\varphi_2,\varphi_1\rangle=\langle\varphi_1,\varphi_2\rangle+\overline{\langle\varphi_1,\varphi_2\rangle}\\ &= 2\mathrm{Re}(\langle\varphi_1,\varphi_2\rangle)\end{aligned}$$

Analogously we compute

$$\|U(t)\varphi_1+U(t)\varphi_2\|_{L^2}^2-\|U(t)\varphi_1\|_{L^2}^2-\|U(t)\varphi_2\|_{L^2}^2=2\mathrm{Re}(\langle U(t)\varphi_1,U(t)\varphi_2\rangle)$$

This and (U1) implies

$$\begin{aligned}2\mathrm{Re}(\langle U(t)\varphi_1,U(t)\varphi_2\rangle) &= \|U(t)\varphi_1+U(t)\varphi_2\|_{L^2}^2-\|U(t)\varphi_1\|_{L^2}^2-\|U(t)\varphi_2\|_{L^2}^2\\ &= \|U(t)(\varphi_1+\varphi_2)\|_{L^2}^2-\|U(t)\varphi_1\|_{L^2}^2-\|U(t)\varphi_2\|_{L^2}^2\\ &\underset{\text{(U1)}}{=} \|\varphi_1+\varphi_2\|_{L^2}^2-\|\varphi_1\|_{L^2}^2-\|\varphi_2\|_{L^2}^2=2\mathrm{Re}(\langle\varphi_1,\varphi_2\rangle).\end{aligned}$$

So, we already find

$$\mathrm{Re}(\langle U(t)\varphi_1,U(t)\varphi_2\rangle)=\mathrm{Re}(\langle\varphi_1,\varphi_2\rangle).$$

Repeating the computation with $i\varphi_1$ in place of φ_1 we find

$$\mathrm{Re}(\langle U(t)(i\varphi_1),U(t)\varphi_2\rangle)=\mathrm{Re}(\langle i\varphi_1,\varphi_2\rangle),$$

i.e.

$$\mathrm{Re}(i\langle U(t)\varphi_1,U(t)\varphi_2\rangle)=\mathrm{Re}(i\langle\varphi_1,\varphi_2\rangle).$$

This accounts for the fact that

$$\mathrm{Im}(\langle U(t)\varphi_1,U(t)\varphi_2\rangle)=\mathrm{Im}(\langle\varphi_1,\varphi_2\rangle),$$

which finishes the proof.

Not only the evolution operator of the Schrödinger equation has properties (U1),(U2),(U3). There are multiple other examples of unitary one-parameter groups.

Example 3.2.5

Let $d=1$ and define the operator family $(U(t):L^2(\mathbb{R};\mathbb{C})\to L^2(\mathbb{R};\mathbb{C}))_{t\in\mathbb{R}}$ as follows. For $\varphi\in L^2(\mathbb{R}^d;\mathbb{C})$ and $t\in\mathbb{R}$ we set

$$(U(t)\varphi)(x):=\varphi(x-t).$$

Claim. $(U(t))_{t\in\mathbb{R}}$ is an SCU-group.

Note first that for any $t \in \mathbb{R}$ the operator $U(t)$ is well defined, as $\psi \in L^2(\mathbb{R};\mathbb{C})$ implies also that $\psi(\cdot - t) \in L^2(\mathbb{R};\mathbb{C})$ (see also derivation of (U1)). Next we derive (U1),(U2),(U3).

- Ad (U1). For $t \in \mathbb{R}$ and $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ we have

$$\|U(t)\varphi\|_{L^2}^2 = \|\varphi(\cdot - t)\|_{L^2}^2 = \int_{\mathbb{R}} |\varphi(x-t)|^2 \,\mathrm{d}x = \int_{\mathbb{R}} |\varphi(y)|^2 \,\mathrm{d}y = \|\varphi\|_{L^2}^2,$$

  where we used the substituion $y = x - t$ in the second to last step. (U1) follows.

- Ad (U2). This is not as easy as it might appear. Indeed, we have to show that

$$\lim_{t\to 0} \int_{\mathbb{R}} |\varphi(x-t) - \varphi(x)|^2 \,\mathrm{d}x = 0 \qquad \text{for all } \varphi \in L^2(\mathbb{R};\mathbb{C}).$$

  First assume that $\varphi \in C_0^\infty(\mathbb{R};\mathbb{C})$. Then clearly $|\varphi(\cdot - t) - \varphi(\cdot)|^2$ converges to zero pointwise as $t \to 0$. Moreover, if $n \in \mathbb{N}$ is such that $\mathrm{spt}(\varphi) \subset (-n, n)$ we have for each $t \in (-1,1)$ that $\mathrm{spt}(\varphi(\cdot - t)) \subset (-(n+1),(n+1))$. This implies that for all $t \in (-1,1)$ and $x \in \mathbb{R}$ we have

$$|\varphi(x-t) - \varphi(x)|^2 \leqslant 2 \max_{\mathbb{R}} |\varphi| \chi_{(-(n+1),n+1)}(x).$$

  Since the right hand side is independent of t and integrable, we have found a dominating function and infer that

$$\lim_{t\to 0} \int_{\mathbb{R}} |\varphi(x-t)-\varphi(x)|^2 \,\mathrm{d}x = \int_{\mathbb{R}} \lim_{t\to 0} |\varphi(x-t)-\varphi(x)|^2 \,\mathrm{d}x = \int_{\mathbb{R}} 0 \,\mathrm{d}x = 0 \;\forall \varphi \in C_0^\infty(\mathbb{R};\mathbb{C}).$$

  We must now prove the same formula for arbitrary $\varphi \in L^2(\mathbb{R};\mathbb{C})$. To this end let $\varepsilon > 0$. Recall from Exercise 4 on Sheet 1 in part III that there exists $\varphi_\varepsilon \in C_0^\infty(\mathbb{R};\mathbb{C})$ such that $\|\varphi - \varphi_\varepsilon\|_{L^2} < \frac{1}{2}\varepsilon$. Now we have

$$\begin{aligned}
\|U(t)\varphi - \varphi\|_{L^2} &= \|U(t)\varphi - U(t)\varphi_\varepsilon + U(t)\varphi_\varepsilon - \varphi_\varepsilon + \varphi_\varepsilon - \varphi\|_{L^2} \\
&\leqslant \|U(t)\varphi - U(t)\varphi_\varepsilon\|_{L^2} + \|U(t)\varphi_\varepsilon - \varphi_\varepsilon\|_{L^2} + \|\varphi_\varepsilon - \varphi\|_{L^2} \\
&= \|U(t)(\varphi - \varphi_\varepsilon)\|_{L^2} + \|U(t)\varphi_\varepsilon - \varphi_\varepsilon\|_{L^2} + \|\varphi_\varepsilon - \varphi\|_{L^2}
\end{aligned}$$

  Using (U1) in the first summand we obtain

$$\|U(t)\varphi - \varphi\|_{L^2} \leqslant 2\|\varphi_\varepsilon - \varphi\|_{L^2} + \|U(t)\varphi_\varepsilon - \varphi_\varepsilon\|_{L^2} \leqslant 2 \cdot (\tfrac{1}{2}\varepsilon) + \|U(t)\varphi_\varepsilon - \varphi_\varepsilon\|_{L^2}$$

  As a result we obtain

$$\limsup_{t\to 0} \|U(t)\varphi - \varphi\|_{L^2} \leqslant \varepsilon + \limsup_{t\to 0} \|U(t)\varphi_\varepsilon - \varphi_\varepsilon\|_{L^2} = \varepsilon,$$

where we have used in the last step that the claim is already shown for functions in $C_0^\infty(\mathbb{R};\mathbb{C})$. Since $\varepsilon > 0$ was arbitrary we obtain that

$$\limsup_{t\to 0} \|U(t)\varphi - \varphi\|_{L^2} = 0,$$

and (U2) follows.

- Ad (U3). This is relatively straightforward. For $\varphi \in L^2(\mathbb{R};\mathbb{C})$ and a.e. $x \in \mathbb{R}^d$ we have

$$\begin{aligned}((U(t)\circ U(s))\varphi)(x) &= U(t)(U(s)\varphi)(x) \\ &= U(t)(\varphi(\cdot - s))(x) = \varphi(\cdot - s)(x-t) = \varphi(x-t-s) \\ &= \varphi(x-(t+s)) = U(t+s)(\varphi)(x).\end{aligned}$$

The claim is shown

Before we close this section a warning: In the following we will often have to distinguish between different types of limits of sequences of L^2-functions. Recall that we have already introduced a precise notation for the L^2-limit: If $(\varphi_n)_{n\in\mathbb{N}} \subset L^2(\mathbb{R}^d;\mathbb{C})$ is a sequence of functions we say $\operatorname*{LIM}_{n\to\infty} \varphi_n = \varphi$ if $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$.

3.2.1 Generators

Our task in the following will be to find the one strongly continuous parameter group that is associated to the Schrödinger equation. To this end we have to introduce the concept of a *generator*.

Definition 3.2.6 — Generator

Let $(U(t))_{t\in\mathbb{R}}$ be an SCU-group. Define

$$D(H) := \{\varphi \in L^2(\mathbb{R}^d;\mathbb{C}) : (\tfrac{U(h)\varphi-\varphi}{h})_{h\in\mathbb{R}\setminus\{0\}} \text{ has a limit in } L^2(\mathbb{R}^d;\mathbb{C}) \text{ as } h \to 0\}$$

and call the *operator* $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ via

$$H\varphi := i \cdot \operatorname*{LIM}_{h\to 0} \frac{U(h)\varphi - \varphi}{h}$$

(where the limit $\operatorname*{LIM}_{h\to 0}$ is to be understood as L^2-limit of functions in $L^2(\mathbb{R}^d;\mathbb{C})$) the *generator* of $(U(t))_{t\in\mathbb{R}}$.

The generator is exactly the right object if one wants to associate a PDE to a SCU-group.

Proposition 3.2.7

Let $(U(t))_{t\in\mathbb{R}}$ be an SCU-group with generator $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$. Further, let

$\varphi \in D(H)$. Then

(i) $t \mapsto U(t)\varphi$ is a differentiable map from $\mathbb{R}$ to $L^2(\mathbb{R}^d;\mathbb{C})$, i.e. there exists $\frac{d}{dt}U(t)\varphi := \operatorname*{LIM}_{h\to 0} \frac{U(t+h)\varphi - U(t)\varphi}{h}$.

(ii) $i\frac{d}{dt}U(t)\varphi = U(t)H\varphi$.

Proof. Let $\varphi \in D(H)$ and $t \in \mathbb{R}$ be arbitrary. We must prove that the L^2-limit

$$\operatorname*{LIM}_{h\to 0}\frac{U(t+h)\varphi - U(t)\varphi}{h}$$

exists. To this end note that

$$\frac{U(t+h)\varphi - U(t)\varphi}{h} = \frac{U(t)(U(h)\varphi) - U(t)\varphi}{h} = U(t)\left(\frac{U(h)\varphi - \varphi}{h}\right)$$

Now observe that $\frac{U(h)\varphi-\varphi}{h} \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} \frac{1}{i}H\varphi$ as $h \to 0$. Since $U(t) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is continuous (as it is an isometry) we have

$$\operatorname*{LIM}_{h\to 0} U(t)\left(\frac{U(h)\varphi - \varphi}{h}\right) = U(t)\left(\operatorname*{LIM}_{h\to 0}\frac{U(h)\varphi - \varphi}{h}\right) = U(t)(\tfrac{1}{i}H\varphi) = \frac{1}{i}U(t)H\varphi.$$

This yields

$$\frac{d}{dt}U(t)\varphi = \operatorname*{LIM}_{h\to 0}\frac{U(t+h)\varphi - U(t)\varphi}{h} = \frac{1}{i}U(t)H\varphi$$

and hence the claim follows.

We discuss now some important basic properties of generators

Proposition 3.2.8

Let $(U(t))_{t\in\mathbb{R}}$ be an SCU-group with generator $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$. Then

(i) For each $t \in \mathbb{R}$ we have $U(t)D(H) = D(H)$

(ii) For each $\varphi \in D(H)$ we have

$$[H, U(t)]\varphi := HU(t)\varphi - U(t)H\varphi = 0$$

(iii) H is symmetric, i.e. for all $\varphi_1, \varphi_2 \in D(H)$ there holds

$$\langle H\varphi_1, \varphi_2\rangle = \langle \varphi_1, H\varphi_2\rangle.$$

Proof. We leave (i) as an exercise, which follows directly from (U3) and the definition of $D(H)$. Ad (ii). Let $\varphi \in D(H)$. Due to (i) we have $U(t)\varphi \in D(H)$ and thus

$$\begin{aligned} HU(t)\varphi &= i\underset{h\to 0}{\mathrm{LIM}}\frac{U(h)U(t)\varphi - U(t)\varphi}{h} = i\underset{h\to 0}{\mathrm{LIM}}\frac{U(t+h)\varphi - U(t)\varphi}{h} \\ &= i\underset{h\to 0}{\mathrm{LIM}}\frac{U(t)U(h)\varphi - U(t)\varphi}{h} = i\underset{h\to 0}{\mathrm{LIM}}\, U(t)\left(\frac{U(h)\varphi - \varphi}{h}\right) \\ &= U(t)\left(i\underset{h\to 0}{\mathrm{LIM}}\,\frac{U(h)\varphi - \varphi}{h}\right) = U(t)H\varphi, \end{aligned}$$

where we used the continuity of to operator $U(t) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ in the second-to last step (which is true as isometries are always continous).

Ad (iii). Let $\varphi_1, \varphi_2 \in D(H)$. Unitariness of $U(t)$ yields (cf. Remark 3.2.4)

$$\langle \varphi_1, \varphi_2\rangle = \langle U(t)\varphi_1, U(t)\varphi_2\rangle.$$

Now we can take the t-derivative on both sides and obtain (with Proposition 3.2.7)

$$\begin{aligned} 0 = \frac{d}{dt}\langle \varphi_1, \varphi_2\rangle &= \frac{d}{dt}\langle U(t)\varphi_1, U(t)\varphi_2\rangle \\ &= \langle \tfrac{d}{dt}U(t)\varphi_1, U(t)\varphi_2\rangle + \langle U(t)\varphi_1, \tfrac{d}{dt}U(t)\varphi_2\rangle \\ &= \langle -iU(t)H\varphi_1, U(t)\varphi_2\rangle + \langle U(t)\varphi_1, -iU(t)H\varphi_2\rangle \\ &= -i\langle U(t)H\varphi_1, U(t)\varphi_2\rangle + \overline{-i}\langle U(t)\varphi_1, U(t)H\varphi_2\rangle \\ &= -i\langle U(t)H\varphi_1, U(t)\varphi_2\rangle + i\langle U(t)\varphi_1, U(t)H\varphi_2\rangle \\ &= i\left(\langle U(t)\varphi_1, U(t)H\varphi_2\rangle - \langle U(t)H\varphi_1, U(t)\varphi_2\rangle\right) \\ &= i\left(\langle \varphi_1, H\varphi_2\rangle - \langle H\varphi_1, \varphi_2\rangle\right), \end{aligned}$$

where we used the unitariness from Remark 3.2.4 again in the last step. We infer that

$$\langle \varphi_1, H\varphi_2\rangle = \langle H\varphi_1, \varphi_2\rangle.$$

Remark 3.2.9 — Associated PDE to a SCU-Group

If we have a SCU-group $(U(t))_{t\in\mathbb{R}}$ with generator $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ given, and if we fix some $\psi_0 \in D(H)$ we may form the function $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C}), t \mapsto U(t)\psi_0$. We can now compute

$$i\frac{d}{dt}\psi = i\frac{d}{dt}U(t)\psi_0 \underset{\text{Prop 3.2.7 (ii)}}{=\!=\!=\!=} U(t)H\psi_0 \underset{\text{Prop 3.2.8 (ii)}}{=\!=\!=\!=} HU(t)\psi_0 = H\psi.$$

In particular we have a solution of

$$i\frac{d}{dt}\psi = H\psi. \tag{43}$$

This yields an *associated equation* to a strongly continous one parameter group.

By definition it is clear that a one parameter group determines its generator $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ uniquely. Hence the associated equation (43) is also uniquely determined by the one parameter group. But does also the generator H determine a one-parameter group uniquely? The answer is (under certain conditions on H) yes! And this is very helpful. Indeed: This allows us to go from an equation like (43) to the associated one parameter group $(U(t))_{t\in\mathbb{R}}$. This is a huge advantage since the equation (43) can only be written down for functions in $D(H)$, while the one parameter group can be evaluated the the wole of $L^2(\mathbb{R}^d;\mathbb{C})$. An important result in this direction is the following

Proposition 3.2.10

Let $(U(t))_{t\in\mathbb{R}}$ be a SCU-group with generator $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$. Further suppose that $D(H)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$.[a] Then H determines $(U(t))_{t\in\mathbb{R}}$ uniquely. More precisely, if $(\tilde{U}(t))_{t\in\mathbb{R}}$ is a SCU-group with generator H then $\tilde{U}(t) = U(t)$ for all $t \in \mathbb{R}$.

[a] That means: For each $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ and $\varepsilon > 0$ one can find $\varphi_\varepsilon \in D(H)$ such that $\|\varphi - \varphi_\varepsilon\|_{L^2} < \varepsilon$.

Proof. Let $t_0 \in \mathbb{R}$ be arbitrary and $(U(t))_{t\in\mathbb{R}}$, $(\tilde{U}(t))_{t\in\mathbb{R}}$ be as in the statement. Further let $\varphi \in D(H)$. We first compute with scalar product identities

$$\begin{aligned}\|U(t)\varphi - \tilde{U}(t)\varphi\|_{L^2}^2 &= \|U(t)\varphi\|_{L^2}^2 + \|\tilde{U}(t)\varphi\|_{L^2}^2 + 2\mathrm{Re}(\langle U(t)\varphi, \tilde{U}(t)\varphi\rangle)\\ &= \|\varphi\|_{L^2}^2 + \|\varphi\|_{L^2}^2 + 2\mathrm{Re}(\langle U(t)\varphi, \tilde{U}(t)\varphi\rangle),\end{aligned}$$

where we have used the unitariness in the last step. Taking now the t-derivative we obtain

$$\begin{aligned}\frac{d}{dt}\|U(t)\varphi - \tilde{U}(t)\varphi\|_{L^2}^2 &= 2\frac{d}{dt}\mathrm{Re}(\langle U(t)\varphi, \tilde{U}(t)\varphi\rangle)\\ &= 2\mathrm{Re}(\langle \tfrac{d}{dt}(U(t)\varphi), \tilde{U}(t)\varphi\rangle + \langle U(t)\varphi, \tfrac{d}{dt}(\tilde{U}(t)\varphi)\rangle)\\ &= 2\mathrm{Re}(\langle -iU(t)H\varphi, \tilde{U}(t)\varphi\rangle + \langle U(t)\varphi, -i\tilde{U}(t)H\varphi\rangle)\\ &= 2\mathrm{Re}(-i\langle U(t)H\varphi, \tilde{U}(t)\varphi\rangle + \overline{-i}\langle U(t)\varphi, \tilde{U}(t)H\varphi\rangle)\\ &\underset{\text{Prop3.2.8(ii)}}{=\!=\!=\!=} 2\mathrm{Re}(-i\langle HU(t)\varphi, \tilde{U}(t)\varphi\rangle + i\langle U(t)\varphi, H\tilde{U}(t)\varphi\rangle)\end{aligned}$$

If we now use the symmetry of H (see Proposition 3.2.8 (iii)) we obtain that the term on the right hand side yields 0 for each $t \in \mathbb{R}$. Hence we have for each $t \in \mathbb{R}$

$$\|U(t)\varphi - \tilde{U}(t)\varphi\|_{L^2}^2 = \|U(0)\varphi - \tilde{U}(0)\varphi\|_{L^2}^2 = \|\varphi - \varphi\|_{L^2} = 0.$$

Putting $t = t_0$ we infer that

$$U(t_0)\varphi = \tilde{U}(t_0)\varphi \qquad \forall \varphi \in D(H). \tag{44}$$

We would like to show that this equality holds actually true for all $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. Let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. Due to the fact that $D(H)$ is dense we can find $(\varphi_n)_{n\in\mathbb{N}} \subset D(H)$ such that $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$. As a result we have by continuity of $U(t_0) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $\tilde{U}(t_0) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$

$$\begin{aligned} U(t_0)\varphi = U(t_0)\left(\operatorname*{LIM}_{n\to\infty} \varphi_n\right) &= \operatorname*{LIM}_{n\to\infty} \left(U(t_0)\varphi_n\right) \\ &\underset{(44)}{=} \operatorname*{LIM}_{n\to\infty} \left(\tilde{U}(t_0)\varphi_n\right) = \tilde{U}(t_0)\left(\operatorname*{LIM}_{n\to\infty} \varphi_n\right) = \tilde{U}(t_0)\varphi. \end{aligned}$$

The claim follows.

With other words: If $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ is an operator such that $D(H)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$ then H generates *at maximum one* SCU-group $(U(t))_{t\in\mathbb{R}}$. Of course we don't know yet whether a given linear operator $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ is at all a generator of an SCU-group (we will see conditions for that in the sequel). But what we do know is that there can be only one SCU-group generated by H. This allows us to give this SCU-group a name.

Definition 3.2.11 — Operator Exponential

Suppose that $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ is a linear operator such that $D(H)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$. Further suppose that $(U(t))_{t\in\mathbb{R}}$ is a SCU-group with generator H. Then we denote

$$U(t) =: e^{-itH}$$

for each $t \in \mathbb{R}$.

The notation is of course motivated by the PDE in Remark 3.2.9. Recall that $\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C}), \psi(t) := e^{-iHt}\psi_0$ solves $i\frac{d}{dt}\psi = H\psi$ if $\psi_0 \in D(H)$. If we multiply with $-i$ we have $\frac{d}{dt}\psi = -iH\psi$, which leads to the natural formula

$$\frac{d}{dt}e^{-itH}\psi_0 = -iHe^{-itH}\psi_0 \qquad \forall t \in \mathbb{R}$$

While this simply looks like the chain rule there are some caveats.

- We have to require that $\psi_0 \in D(H)$ to write down this formula
- e^{-iHt} is an operator defined on the whole of $L^2(\mathbb{R}^d;\mathbb{C})$. It would be desirable to approximate it numerically. One idea how this could be achieved is by means of the *series representation of the exponential function*

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} \qquad \forall x \in \mathbb{R}$$

However, such a series representation does not meaningfully carry over in our infinite-dimensional setting! Indeed, if one would formally insert $-iHt$ in place of x in the above equation one would have to evaluate powers of the form H^k, $k \in \mathbb{N}_0$. But in order evaluate H^k one has to be in the domain $D(H^k)$ which is not necessarily the whole of $L^2(\mathbb{R}^d; \mathbb{C})$ and possibly not even dense there (see Exercise sheet 1, Exercise 1c).

– Nevertheless, it is a rich field of research to study how one can approximate e^{-iHt} numerically. One could fill multiple lectures with that. We will not go into details here (but we will do a little bit of theory on matrix exponentials in the next section).

We will now get back to our Schrödinger equation with potential V given by

$$i\frac{d}{dt}\psi = -\frac{1}{2}\Delta_x\psi + V\psi$$

This suggests an operator of the form $H : D(H) \to L^2(\mathbb{R}^d; \mathbb{C})$ such that

$$H\psi = -\frac{1}{2}\Delta_x\psi + V\psi$$

for all $\psi \in D(H)$ (where $D(H)$ is yet to be chosen).

Question. Does such an operator H generate a SCU-group?

We already know that there are some necessary criteria that H needs to satisfy. Indeed, e.g. from Proposition 3.2.8 (iii) we learn that each operator that can possibly generate a SCU-group must necessarily be symmetric. But is this symmetry also sufficient? Unfortunately not!
Mathematical literature has a very beautiful theorem for us, which even presents a *necessary and sufficient condition* for the generation of a SCU-group.

Theorem 3.2.12 — Stone's Theorem

Suppose that $H : D(H) \to L^2(\mathbb{R}^d; \mathbb{C})$ is a linear operator such that $D(H)$ is dense in $L^2(\mathbb{R}^d; \mathbb{C})$. Then the following two assertions are equivalent

(a) H generates a SCU-group $(e^{-itH})_{t\in\mathbb{R}}$

(b) H is *self-adjoint* (see Definition 3.2.13 below)

Proof. Goes beyond the scope of this lecture.

Once we accept this theorem, we have an easy time answering the question posed above. We just have to check, whether te operator H is self-adjoint. But before we can do so, we first have to discuss the concept of self-adjointness in detail. We shall do so in the coming section.

3.2.2 Self-Adjointness

First of all I owe you the definition of self-adjointness. But before giving this definition I would like to point out a caveat: Recall that matrix $M \in \mathbb{C}^{n\times n}$ is called self-adjoint (or Hermitean symmetric) if $\overline{M}^T = M$. We have already seen in the discussion below Definition 2.1.4 that this corresponds to *symmetry* of the operator $A : \mathbb{C}^n \to \mathbb{C}^n, x \mapsto M \cdot x$. In particular, in finite dimension the notions of self-adjointness and (Hermitean) symmetry coincide. However (and this is the caveat I would like to stress), in infinite dimension *self-adjointness is a stronger concept than symmetry.* This is mainly due to the fact that

Definition 3.2.13 — Self-Adjointness

Let $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ be a linear operator such that $D(H)$ is dense. We call H *self-adjoint*[a] if

(i) H is symmetric, i.e. $\langle H\varphi_1, \varphi_2\rangle = \langle \varphi_1, H\varphi_2\rangle$ for all $\varphi_1, \varphi_2 \in D(H)$

(ii) The domain $D(H)$ satisfies

$$\{f \in L^2(\mathbb{R}^d;\mathbb{C}) : \exists C > 0 \text{ s.t. } |\langle H\varphi, f\rangle| \leqslant C\|\varphi\|_{L^2}\ \forall \varphi \in D(H)\} \subseteq D(H). \tag{45}$$

[a]If we do not assume that $D(H)$ is dense, the canonical definition in the literature would be slightly different. We use here the definition that is most convenient for us.

Condition (ii) looks somewhat counterintuitive at first sight, but we will try to shed some light on it now. Let $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ be an operator which is (for now only symmetric). Suppose we have $\varphi \in D(H)$ and $f \in L^2(\mathbb{R}^d;\mathbb{C})$ and we form the expression

$$\langle H\varphi, f\rangle$$

Since H is symmetric, we know that if $f \in D(H)$ we can shift H to f and reformulate it as $\langle \varphi, Hf\rangle$. In this case we have

$$|\langle H\varphi, f\rangle| = |\langle \varphi, Hf\rangle| \leqslant \|Hf\|_{L^2}\|\varphi\|_{L^2}.$$

In particular, each $f \in D(H)$ lies in the set on the left hand side of (45). In particular this shows that in (45) the set inclusion "$\supseteq$" is true simply due to the symmetry.
The fact that "$\subseteq$" therefore yields an exact requirement on the domain $D(H)$.

Remark 3.2.14

We would like to attempt another explanation of (45). Suppose that $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ is symmetric and such that $D(H)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$. Suppose that $f \in L^2(\mathbb{R}^d;\mathbb{C})$ is such that

$$|\langle H\varphi, f\rangle| \leqslant C\|\varphi\|_{L^2} \qquad \text{for all } \varphi \in D(H), \tag{46}$$

i.e. f lies in the set on the left hand side of (45).

Claim. There exists $g \in L^2(\mathbb{R}^d;\mathbb{C})$ such that $\langle H\varphi, f\rangle = \langle \varphi, g\rangle$ for all $\varphi \in D(H)$.

Before we prove this, let us discuss what it means. It means that for each f in the set of the left hand side of (45) we are allowed to pull H to the other side of the scalar product. Due to the symmetry of H we would actually expect that $g = Hf$, but this is only ensured if $f \in D(H)$. Thankfully, this is exactly what the self-adjointness requirement (ii) provides: If (46) is satisfied, then we already have $f \in D(H)$ and shifting the operator away to the other side is allowed.

Proof. (!Functional Analysis!) Define $F : D(H) \to \mathbb{R}$ via $F(\varphi) := \langle H\varphi, f\rangle$.

Intermediate claim. F can be extended to a continuous linear operator $\bar{F} : L^2(\mathbb{R}^d;\mathbb{C}) \to \mathbb{C}$.

To this end let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. Then there exists a sequence $(\varphi_n)_{n\in\mathbb{N}} \subset D(H)$ such that $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$. Since for all $m, n \in \mathbb{N}$ we have

$$|F(\varphi_n) - F(\varphi_m)| = |F(\varphi_n - \varphi_m)| \leqslant C\|\varphi_n - \varphi_m\|_{L^2}$$

we obtain that $(F(\varphi_n))_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathbb{R}$ and hence a reasonable choice for $\bar{F}(\varphi)$ is $\bar{F}(\varphi) = \lim_{n\to\infty} F(\varphi_n)$. To make sure that this is well-defined, we have to ensure that this number does not depend on the chosen sequence $(\varphi_n)_{n\in\mathbb{N}}$. This is readily checked: If $(\varphi_n)_{n\in\mathbb{N}}, (\eta_n)_{n\in\mathbb{N}}$ are two sequences that converge to φ we obtain that

$$|F(\varphi_n) - F(\eta_n)| \leqslant C\|\varphi_n - \eta_n\|_{L^2} \leqslant C(\|\varphi_n - \varphi\|_{L^2} + \|\varphi - \eta_n\|_{L^2}) \xrightarrow{n\to\infty} C \cdot (0 + 0) = 0.$$

This implies that

$$\lim_{n\to\infty} F(\varphi_n) = \lim_{n\to\infty} F(\eta_n)$$

and thus our definition of $\bar{F}(\varphi)$ is well-defined. We leave it as an exercise to show that $\bar{F}$ is linear. It remains to show continuity (equivalently boundedness) of $\bar{F}$. To this end let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ and choose $(\varphi_n)_{n\in\mathbb{N}} \subset D(H)$ such that $\varphi_n \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} \varphi$. Then the definition of $\bar{F}$ yields $\bar{F}(\varphi) = \lim_{n\to\infty} F(\varphi_n)$. Thus we have

$$|\bar{F}(\varphi)| = \lim_{n\to\infty} |F(\varphi_n)| \leqslant \limsup_{n\to\infty} C\|\varphi_n\|_{L^2} = C\|\varphi\|_{L^2},$$

where we have used continuity of the L^2-Norm with respect to L^2-convergence.[a] The intermediate claim is shown.

End of intermediate claim.

Now the claim follows easily: Since $\bar{F}$ is a continus linear functional on $L^2(\mathbb{R}^d;\mathbb{C})$, the Riesz representation theorem yields that there exists some $g \in L^2(\mathbb{R}^d;\mathbb{C})$ such that

$$\bar{F}(\varphi) = \langle \varphi, g\rangle \qquad \forall \varphi \in L^2(\mathbb{R}^d;\mathbb{C}).$$

As a result we have for each $\varphi \in D(H)$

$$\langle H\varphi, f\rangle = F(\varphi) = \bar{F}(\varphi) = \langle \varphi, g\rangle$$

[a] Recall: This is actually an easy consequence of the inverse triangle inequality

$$|\,\|\varphi_n\|_{L^2} - \|\varphi\|_{L^2}\,| \leqslant \|\varphi_n - \varphi\|_{L^2} \xrightarrow{n\to\infty} 0.$$

Next we see some useful examples of self-adjoint operators.

Example 3.2.15 — Self-Adjointness of multiplication operators

Let $V : \mathbb{R}^d \to \mathbb{R}$ be a measurable and real-valued function. Set

$$D(M_V) := \{f \in L^2(\mathbb{R}^d, \mathbb{C}) : Vf \in L^2(\mathbb{R}^d; \mathbb{C})\}$$

and define $M_V : D(M_V) \to L^2(\mathbb{R}^d; \mathbb{C})$ to be

$$M_V\varphi := V \cdot \varphi$$

Claim. M_V is self-adjoint.

Proof. First we check the symmetry (Point (i) in Definition 3.2.13). Let $f, g \in D(M_V)$. Then

$$\langle Vf, g\rangle = \int_{\mathbb{R}^d} V(x)f(x)\overline{g(x)}\,\mathrm{d}x = \int_{\mathbb{R}^d} \overline{V(x)}f(x)\overline{g(x)}\,\mathrm{d}x = \int_{\mathbb{R}^d} f(x)\overline{V(x)g(x)}\,\mathrm{d}x = \langle f, Vg\rangle.$$

Here we have used extensively that V is real-valued. Now we proceed with Point (ii) in Definition 3.2.13. Suppose that $f \in L^2(\mathbb{R}^d; \mathbb{C})$ is such that there exists $C > 0$ with the property that

$$\langle M_V\varphi, f\rangle \leqslant C\|\varphi\|_{L^2} \text{ for all } \varphi \in D(M_V). \qquad (*).$$

We need to show that $f \in D(M_V)$, i.e. $Vf \in L^2(\mathbb{R}^d; \mathbb{C})$. To this end let $n \in \mathbb{N}$ be arbitrary and define

$$V_n : \mathbb{R}^d \to \mathbb{R}, \quad V_n(x) := \begin{cases} V(x) & |V(x)| \leqslant n \\ 0 & \text{otherwise} \end{cases}. \tag{47}$$

Notice that $\varphi_n := V_n f$ lies in $D(M_V)$. Indeed, firstly one has

$$|\varphi_n| = |V_n f| = |V_n|\,|f| \leqslant n|f| \in L^2(\mathbb{R}^d; \mathbb{C}),$$

and secondly (since $VV_n = V_n^2$, as one readily checks with (47))

$$|V\varphi_n| = |VV_n f| = |V_n^2 f| = |V_n|^2\,|f| \leqslant n^2|f| \in L^2(\mathbb{R}^d; \mathbb{C}).$$

Therefore we have $\langle M_V\varphi_n, f\rangle \leqslant C\|\varphi_n\|_{L^2}$. Now we compute

$$\begin{aligned}\langle M_V\varphi_n, f\rangle &= \int_{\mathbb{R}^d} V(x)\varphi_n(x)\overline{f(x)}\,\mathrm{d}x = \int_{\mathbb{R}^d} V(x)V_n(x)f(x)\overline{f(x)}\,\mathrm{d}x\\ &= \int_{\mathbb{R}^d} V_n(x)^2|f(x)|^2\,\mathrm{d}x = \|V_n f\|_{L^2}^2 = \|\varphi_n\|_{L^2}^2.\end{aligned}$$

This yields that $\|\varphi_n\|_{L^2}^2 \leqslant C\|\varphi_n\|_{L^2}$ and thus $\|\varphi_n\|_{L^2} \leqslant C$ for all $n \in \mathbb{N}$. In particular

$$\int_{\mathbb{R}^d} |\varphi_n(x)|^2\,\mathrm{d}x \leqslant C^2 \qquad \text{for all } n \in \mathbb{N} \tag{48}$$

Now observe that $V_n \xrightarrow{\text{ptw.}} V$ as $n \to \infty$. For this reason we have (by Fatou's Lemma, see Satz 2.2.9 in ↑ `Analysis III Lecture Notes`)

$$\begin{aligned}\int_{\mathbb{R}^d} |V(x)f(x)|^2\,\mathrm{d}x &= \int_{\mathbb{R}^d} \liminf_{n\to\infty} |V_n(x)f(x)|^2\,\mathrm{d}x \leqslant \liminf_{n\to\infty}\int_{\mathbb{R}^d} |V_n(x)f(x)|^2\,\mathrm{d}x\\ &= \liminf_{n\to\infty}\int_{\mathbb{R}^d} |\varphi_n(x)|^2\,\mathrm{d}x \underset{(48)}{\leqslant} C^2.\end{aligned}$$

This implies that $Vf \in L^2(\mathbb{R}^d;\mathbb{C})$ and hence $f \in D(H)$. The claim is shown.

Since M_V is self-adjoint it must (according to Theorem 3.2.12) also generate a SCU-group. It is an exercise to show that the group generated by M_V is given by $(U_V(t))_{t\in\mathbb{R}}$ defined by

$$U_V(t) : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C}), \quad (U_V(t)\varphi)(x) := e^{-iV(x)t}\varphi(x) \quad \text{a.e. } x \in \mathbb{R}^d.$$

While this seems very canonical the devil is in the details, especially since one must be careful to not confuse pointwise limits of functions with L^2-limits of functions. (Definition 3.2.6 works with the latter concept, while our intuition often looks at pointwise limits).

In the coming example we will work with the hogher order Sobolev space $W^{2,2}(\mathbb{R}^d;\mathbb{C})$. Recall that this space can be defined as the set of all function $f \in L^2(\mathbb{R}^d;\mathbb{C})$ such that there exist $g_1, ..., g_d \in L^2(\mathbb{R}^d;\mathbb{C})$ and $h_{jk} \in L^2(\mathbb{R}^d;\mathbb{C})$ $(j,k = 1,...,d)$ such that

$$\int_{\mathbb{R}^d} f\partial_{x_i}\eta\,\mathrm{d}x = -\int_{\mathbb{R}^d} g_i\eta\,\mathrm{d}x \qquad \forall \eta \in C_0^\infty(\mathbb{R}^d;\mathbb{C}),$$

$$\int_{\mathbb{R}^d} f\partial^2_{x_jx_k}\eta\,\mathrm{d}x = -\int_{\mathbb{R}^d} h_{jk}\eta\,\mathrm{d}x \qquad \forall \eta \in C_0^\infty(\mathbb{R}^d;\mathbb{C}).$$

The functions g_i, h_{jk} $(i,j,k \in \{1,...,d\})$ are uniquely determined and are called $g_i =: \partial_{x_i}f$ and $h_{jk} =: \partial^2_{x_jx_k}f$. We would also like to stress that $W^{2,2}(\mathbb{R}^d;\mathbb{C})$ coincides with the space W_2 defined in Definition 10.1 of Part II of this lecture.

Example 3.2.16

Define $D(\Delta) := W^{2,2}(\mathbb{R}^d;\mathbb{C})$ and the Laplacian $\Delta : D(\Delta) \to L^2(\mathbb{R}^d;\mathbb{C})$ via $\Delta\varphi := \sum_{i=1}^d \partial^2_{x_i}\varphi$.

Claim. Δ is self-adjoint.

***Proof.**[a] First we show the symmetry (Condition (i) in Definition 3.2.13). Let $\varphi_1, \varphi_2 \in D(\Delta) = W^{2,2}(\mathbb{R}^d;\mathbb{C})$. Similar to Lemma 2.1.6 one can show that there exists $(\eta_n)_{n\in\mathbb{N}} \subset C_0^\infty(\mathbb{R}^d;\mathbb{C})$ such that

$$\eta_n \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} \varphi_2, \quad \partial_{x_i}\eta_n \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} \partial_{x_i}\varphi_2 \; \forall i = 1, ..., d, \quad \partial_{x_j x_k}\eta_n \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} \partial_{x_j x_k}\varphi_2 \; \forall j, k = 1, ..., d.$$

As a result we have (using multiple times the definition of weak derivative)

$$\begin{aligned}
\langle \Delta\varphi_1, \varphi_2 \rangle &= \int_{\mathbb{R}^d} \Delta\varphi_1(x)\overline{\varphi_2(x)} \, \mathrm{d}x = \lim_{n\to\infty} \int_{\mathbb{R}^d} \Delta\varphi_1(x)\overline{\eta_n(x)} \, \mathrm{d}x \\
&= \lim_{n\to\infty} \sum_{i=1}^d \int_{\mathbb{R}^d} \frac{\partial^2}{\partial x_i^2}\varphi_1(x)\overline{\eta_n(x)} \, \mathrm{d}x = \lim_{n\to\infty} \sum_{i=1}^d \int_{\mathbb{R}^d} \varphi_1(x)\overline{\frac{\partial^2}{\partial x_i^2}\eta_n(x)} \, \mathrm{d}x \\
&= \sum_{i=1}^d \int_{\mathbb{R}^d} \varphi_1(x)\overline{\frac{\partial^2}{\partial x_i^2}\varphi_2(x)} \, \mathrm{d}x = \int_{\mathbb{R}^d} \varphi_1(x)\overline{\Delta\varphi_2(x)} \, \mathrm{d}x = \langle \varphi_1, \Delta\varphi_2 \rangle.
\end{aligned}$$

Now we verify Condition (ii) in Definition 3.2.13. To this end let $f \in L^2(\mathbb{R}^d;\mathbb{C})$ be such that there exists $C > 0$ with the property that

$$|\langle \Delta\varphi, f \rangle| \leqslant C\|\varphi\|_{L^2} \qquad \forall \varphi \in W^{2,2}(\mathbb{R}^d;\mathbb{C}).$$

By Remark 3.2.14 that means that there exists $g \in L^2(\mathbb{R}^d;\mathbb{C})$ such that

$$\langle \Delta\varphi, f \rangle = \langle \varphi, g \rangle \qquad \forall \varphi \in W^{2,2}(\mathbb{R}^d;\mathbb{C}).$$

Since $C_0^\infty(\mathbb{R}^d;\mathbb{R}) \subseteq W^{2,2}(\mathbb{R}^d;\mathbb{C})$ we infer

$$\int_{\mathbb{R}^d} \overline{f(x)}\Delta\varphi(x) \, \mathrm{d}x = \int_{\mathbb{R}^d} \overline{g(x)}\varphi(x) \, \mathrm{d}x \qquad \text{for all } \varphi \in C_0^\infty(\mathbb{R}^d;\mathbb{R}),$$

i.e. $\Delta\overline{f} = \overline{g}$ in the sense of distributions. In particular, we have that $\overline{f} \in L^2(\mathbb{R}^d;\mathbb{C})$ satisfies $\Delta\overline{f} \in L^2(\mathbb{R}^d;\mathbb{C})$. Elliptic regularity of the Laplacian (see Lemma 10.6 (a) in Part II applied with $m = 0$) yields $\overline{f} \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$ and thus clearly also $f \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$. We have this shown that $f \in D(\Delta)$ and the selfadjointness follows.

[a] The proof is optional since we will later see another proof of this fact.

Since $\Delta : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint, we also know that $-\frac{1}{2}\Delta : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint. Hence, $-\frac{1}{2}\Delta$ must again generate an SCU-group. We will next show that this SCU-group $(U(t))_{t\in\mathbb{R}}$ is given precisely via

$$U(t)\varphi := \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)$$

and hence coincides with the SCU-group discussed in Example 3.2.2.

Proposition 3.2.17

Let $(U(t))_{t\in\mathbb{R}}$ be the SCU-group generated by $-\frac{1}{2}\Delta : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$. Then for each $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ and $t \in \mathbb{R}$ we have

$$U(t)\varphi = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi).$$

In our notation we have $e^{-\frac{i}{2}t\Delta}\varphi = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)$ for all $t \in \mathbb{R}$ and $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$.

Proof. Let $(U(t))_{t\in\mathbb{R}}$ be the SCU-group generated by $-\frac{1}{2}\Delta : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$. We show the claim first for $\varphi \in D(\Delta) = W^{2,2}(\mathbb{R}^d;\mathbb{C})$. We let therefore $\varphi \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$. Define

$$\psi : \mathbb{R} \to L^2(\mathbb{R}^d;\mathbb{C}), \qquad t \mapsto \psi_t := U(t)\varphi \tag{49}$$

Intermediate Claim. ψ is a distributional solution of the free Schrödinger equation in the sense of Definition 3.1.4

To this end let $\eta \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. We need to show that

$$i\frac{d}{dt}L_{\psi_t}(\eta) = -\frac{1}{2}L_{\psi_t}(\Delta\eta) \qquad \forall t \in \mathbb{R}$$

To this end we compute by means of Remark 3.2.9[a]

$$\begin{aligned}\frac{d}{dt}L_{\psi_t}(\eta) &= \frac{d}{dt}\langle\psi_t, \bar{\eta}\rangle = \frac{d}{dt}\langle U(t)\varphi, \bar{\eta}\rangle = \langle \tfrac{d}{dt}(U(t)\varphi), \bar{\eta}\rangle \\ &\underset{\text{Rem3.2.9}}{=\!=\!=} \langle -\tfrac{1}{2}\Delta(U(t)\varphi), \eta\rangle \underset{(*)}{=} -\frac{1}{2}\langle U(t)\varphi, \Delta\bar{\eta}\rangle = -\frac{1}{2}\langle\psi_t, \overline{\Delta\eta}\rangle = -\frac{1}{2}L_{\psi_t}(\Delta\eta).\end{aligned}$$

The intermediate claim is shown. Note that in $(*)$ we have used the symmetry of $-\frac{1}{2}\Delta$ as was discussed in Example 3.2.16.

In particular, ψ defined as in (49) solves the distributional free Schrödinger equation and attains the initial value $U(0)\varphi = \varphi$ at $t = 0$. By Theorem 3.1.4 (the uniqueness part) we must have $\psi_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)$ for all $t \in \mathbb{R}$ and thus conclude

$$U(t)\varphi = \psi_t = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi) \qquad \forall t \in \mathbb{R}. \tag{50}$$

This holds now for all $\varphi \in D(\Delta) = W^{2,2}(\mathbb{R}^d;\mathbb{C})$. We would now like to extend this to all $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. To this end let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ and $t \in \mathbb{R}$. Further fix $\varepsilon > 0$ and choose some $\eta \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$ such that $\|\eta - \varphi\|_{L^2} < \varepsilon$. Now, (50) yields

$$U(t)\eta = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\eta).$$

Due to this fact we have

$$\begin{aligned}\|U(t)\varphi - \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)\|_{L^2} &= \|U(t)\varphi + 0 - \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)\|_{L^2} \\ &= \|U(t)\varphi - U(t)\eta + \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\eta) - \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)\|_{L^2} \\ &= \|U(t)(\varphi-\eta) - \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\varphi-\eta))\|_{L^2} \\ &= \|U(t)(\varphi-\eta)\|_{L^2} + \|\mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}(\varphi-\eta))\|_{L^2} \\ &= \|\varphi-\eta\|_{L^2} + \|\varphi-\eta\|_{L^2} \leqslant 2\varepsilon,\end{aligned}$$

where in the last line we have used the isometry properties of $U(t), \mathcal{F}^{-1}$ and $\mathcal{F}$. Since $\varepsilon > 0$ was arbitary we infer

$$\|U(t)\varphi - \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)\|_{L^2} = 0,$$

i.e. $U(t)\varphi = \mathcal{F}^{-1}(e^{-\frac{i}{2}|\cdot|^2 t}\mathcal{F}\varphi)$ for any $t \in \mathbb{R}$. The claim follows.

[a] Notice that in this Remark it is needed that that $\varphi \in D(\Delta)$

Before we proceed to studying the self-adjointness of the Schrödinger operator with potential we would like to formulate a useful criterion for self-adjointness.

Proposition 3.2.18 — Self-Adjointness criterion

Let $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ be a symmetric operator such that $D(H)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$. Further suppose that $H + i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $H - i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ are surjective. Then H is self-adjoint.

Proof. Let $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ be as in the statement. We have to check again point (i) and (ii) in Definition 3.2.13. Point (i) is given in the prerequisite. We therefore turn to (ii). Suppose that $f \in L^2(\mathbb{R}^d;\mathbb{C})$ is such that there exists $C > 0$ with the property that

$$|\langle H\varphi, f\rangle| \leqslant C\|\varphi\|_{L^2} \qquad \text{for all } \varphi \in D(H).$$

We must show that $f \in D(H)$. To this end first note that according to Remark 3.2.14 we can find some $g \in L^2(\mathbb{R}^d;\mathbb{C})$ such that

$$\langle H\varphi, f\rangle = \langle \varphi, g\rangle \quad \forall \varphi \in D(H). \tag{51}$$

Due to the surjectivity of $H - i\mathrm{Id}$ we can find some $\varphi_0 \in D(H)$ such that

$$(H - i\mathrm{Id})\varphi_0 = g - if$$

In particular $g = H\varphi_0 - i\varphi_0 + if = H\varphi_0 + i(f - \varphi_0)$. Using this in (51) we obtain for $\varphi \in D(H)$

$$\langle H\varphi, f\rangle = \langle \varphi, g\rangle = \langle \varphi, H\varphi_0 + i(f - \varphi_0)\rangle = \langle \varphi, H\varphi_0\rangle + (-i)\langle \varphi, f - \varphi_0\rangle.$$

Now we use the symmetry of H and the fact that $\varphi, \varphi_0 \in D(H)$ to obtain

$$\langle H\varphi, f\rangle = \langle H\varphi, \varphi_0\rangle + (-i)\langle \varphi, f - \varphi_0\rangle.$$

Substracting $\langle H\varphi, \varphi_0\rangle$ on both sides we have

$$\langle H\varphi, f - \varphi_0\rangle = (-i)\langle \varphi, f - \varphi_0\rangle$$

And as a result

$$\langle (H + i\mathrm{Id})\varphi, f - \varphi_0\rangle = 0 \qquad \forall \varphi \in D(H). \tag{52}$$

Since also $(H + i\mathrm{Id})$ is surjective on $L^2(\mathbb{R}^d; \mathbb{C})$ we can find some $\varphi_* \in D(H)$ such that $(H + i\mathrm{Id})\varphi_* = f - \varphi_0$. Plugging in φ_* in (52) we obtain

$$0 = \langle (H + i\mathrm{Id})\varphi_*, f - \varphi_0\rangle = \langle f - \varphi_0, f - \varphi_0\rangle = \|f - \varphi_0\|_{L^2}^2.$$

This yields $f = \varphi_0$ (as elements of L^2), i.e. we have $f \in D(H)$ (since $\varphi_0 \in D(H)$). The claim is shown.

Remark 3.2.19

Actually the converse direction in the previous proposition is also true, i.e. if $H : D(H) \to L^2(\mathbb{R}^d; \mathbb{C})$ is self-adjoint then also $H \pm i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d; \mathbb{C})$ are surjective operators. We will not need this result in the sequel, but we give a proof a supplementary material.

***Proof.** (!Functional Analysis!) Let H be self-adjoint. Define $R_\pm := \{H\varphi \pm i\varphi : \varphi \in D(H)\}$. Moreover we define for $M \subseteq L^2(\mathbb{R}^d; \mathbb{C})$ the *orthogonal complement*

$$M^\perp := \{f \in L^2(\mathbb{R}^d; \mathbb{C}) : \langle f, g\rangle = 0 \ \forall g \in M\}.$$

STEP 1. We show that $R_\pm^\perp = \{0\}$ (for the sake of simplicity only with $\pm = +$).

Suppose that $f \in L^2(\mathbb{R}^d; \mathbb{C})$ is such that $f \perp R_+$, i.e.

$$\langle H\varphi + i\varphi, f\rangle = 0 \qquad \text{for all } \varphi \in D(H),$$

in particular $\langle H\varphi, f\rangle = -i\langle \varphi, f\rangle$. The Cauchy-Schwarz inequality yields then

$$|\langle H\varphi, f\rangle| = |\langle \varphi, f\rangle| \leqslant \|\varphi\|_{L^2}\|f\|_{L^2} \qquad \text{for all } \varphi \in D(H).$$

Hence f lies in the set specified on the right hand side of (45) with $C = \|f\|_{L^2}$. We conclude from (45) that $f \in D(H)$. Using this and the symmetry of H in yields that for all $\varphi \in D(H)$

$$0 = \langle H\varphi, f\rangle + i\langle \varphi, f\rangle = \langle \varphi, Hf\rangle + \langle \varphi, -if\rangle = \langle \varphi, Hf - if\rangle.$$

Since $D(H)$ is dense this allows us to conclude that $Hf - if = 0$. Due to the next proposition (Proposition 3.2.20 which is proved independently of our remark above) we have $f = 0$.

Step 2. $\overline{R_\pm} = L^2(\mathbb{R}^d; \mathbb{C})$.

This will follow from Step 1 and the following

Fact. A subset $M \subseteq L^2(\mathbb{R}^d; \mathbb{C})$ with $M^\perp = \{0\}$ must already be dense.

This can be seen as follows. Let $M \subseteq L^2(\mathbb{R}^d; \mathbb{C})$ be such that $M^\perp = \{0\}$. Note that $\overline{M}$ is a closed subspace of $L^2(\mathbb{R}^d; \mathbb{C})$. Hence by standard Hilbert space theory we have $\overline{M} \oplus \overline{M}^\perp = L^2(\mathbb{R}^d; \mathbb{C})$ $(*)$. Moreover, clearly $\overline{M}^\perp \subseteq M^\perp = \{0\}$, so $\overline{M}^C = \{0\}$. This and $(*)$ yields $\overline{M} = L^2(\mathbb{R}^d; \mathbb{C})$ as claimed.

Step 3. $R_\pm = L^2(\mathbb{R}^d; \mathbb{C})$

To this end we show that $R_\pm$ is closed. As a consequence of this and Step 2 we obtain $R_\pm = \overline{R_\pm} = L^2(\mathbb{R}^d; \mathbb{C})$. We focus again only on the case $\pm = +$. Let $(\eta_n)_{n\in\mathbb{N}} \subseteq R_+$ be such that $\eta_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \eta$ for some $\eta \in L^2(\mathbb{R}^d; \mathbb{C})$. We must show that $\eta \in R_+$. For $n \in \mathbb{N}$ let $\varphi_n \in D(H)$ be such that

$$\eta_n = H\varphi_n + i\varphi_n.$$

In particular for $n, m \in \mathbb{N}$ we have $\eta_n - \eta_m = H(\varphi_n - \varphi_m) + i(\varphi_n - \varphi_m)$ and thus

$$\langle \eta_n - \eta_m, \varphi_n - \varphi_m\rangle = \langle \varphi_n - \varphi_m, H(\varphi_n - \varphi_m)\rangle + i\|\varphi_n - \varphi_m\|_{L^2}^2 \tag{53}$$

Note that due to the symmetry of H we have

$$\langle \varphi_n - \varphi_m, H(\varphi_n - \varphi_m)\rangle \in \mathbb{R} \qquad \text{(cf. Remark 2.1.8)},$$

so that (53) yields

$$\|\varphi_n - \varphi_m\|_{L^2}^2 = \operatorname{Im}\langle \eta_n - \eta_m, \varphi_n - \varphi_m\rangle \leqslant |\langle \eta_n - \eta_m, \varphi_n - \varphi_m\rangle| \leqslant \|\eta_n - \eta_m\|_{L^2}\|\varphi_n - \varphi_m\|_{L^2}.$$

As a consequence we have $\|\varphi_n - \varphi_m\|_{L^2} \leqslant \|\eta_n - \eta_m\|_{L^2}$, implying that $(\varphi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence. Since $L^2(\mathbb{R}^d; \mathbb{C})$ is complete we obtain that there exists $\varphi \in L^2(\mathbb{R}^d; \mathbb{C})$ such that $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$. Not just do we have $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$ but also

$$H\varphi_n = \eta_n - i\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \eta - i\varphi.$$

By Lemma 4.0.6(i) (proved independently of the present remark) we have that $\varphi \in D(H)$ and $H\varphi = \eta - i\varphi$. With other words

$$\eta = H\varphi + i\varphi \in R_+.$$

In Proposition 3.2.18 we could have also asked without any additional information as a prerequisite that $H + i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $H - i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ are bijective (and not just surjective). That the injectivity comes for free will be proved in the next proposition.

Proposition 3.2.20

Let $H : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ be a symmetric operator such that $D(H)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$. Then $H + i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $H - i\mathrm{Id} : D(H) \to L^2(\mathbb{R}^d;\mathbb{C})$ are also injective.

Proof. We only show that $H + i\mathrm{Id}$ is injective. To this end we show that the kernel is trivial. Suppose that $\varphi \in D(H)$ is such that $(H + i\mathrm{Id})(\varphi) = 0$. Then we also have

$$0 = \langle (H + i\mathrm{Id})\varphi, \varphi\rangle = \langle H\varphi, \varphi\rangle + i\langle \varphi, \varphi\rangle = \langle H\varphi, \varphi\rangle + i\|\varphi\|^2_{L^2}. \tag{54}$$

Now observe that due to symmetry of H and properties of the scalar product we have $\langle H\varphi, \varphi\rangle = \langle \varphi, H\varphi\rangle = \overline{\langle H\varphi, \varphi\rangle}$, which yields that $\langle H\varphi, \varphi\rangle \in \mathbb{R}$ (cf. Remark 2.1.8). Using this we learn from (54) that

$$0 = \mathrm{Im}(0) = \mathrm{Im}(\langle H\varphi, \varphi\rangle + i\|\varphi\|^2_{L^2}) = \|\varphi\|^2_{L^2},$$

i.e. $\varphi = 0$. This implies that $\ker(H + i\mathrm{Id}) = \{0\}$ and the injectivity is shown.

Example 3.2.21

We now show once again that $-\frac{1}{2}\Delta : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint, but this time by means of the criterion in Proposition 3.2.18. We even check a stronger statement which will come in handy later:

Claim. For any $\mu > 0$ the operator $-\frac{1}{2}\Delta \pm \mu i\mathrm{Id} : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is surjective.[a]

Proof. Let $f \in L^2(\mathbb{R}^d;\mathbb{C})$. All we need to do is find $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$ such that $-\frac{1}{2}\Delta u + \mu i u = f$. We look at the Fourier transform and find that this is equivalent to[b]

$$(\tfrac{1}{2}|p|^2 + i\mu)\mathcal{F}(u)(p) = \mathcal{F}(f)(p) \qquad \text{a.e. } p \in \mathbb{R}^d \tag{55}$$

Can we find some $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$ satisfying this relation?

STEP 1. There exists $u \in L^2(\mathbb{R}^d;\mathbb{C})$ such that $\mathcal{F}(u) = \frac{1}{\frac{1}{2}|\cdot|^2 + i\mu}\mathcal{F}(f)$

To this end note first that $\frac{1}{\frac{1}{2}|\cdot|^2+i\mu}\mathcal{F}(f)$ lies in $L^2(\mathbb{R}^d;\mathbb{C})$. Indeed, we have

$$\begin{aligned}\int_{\mathbb{R}^d}\left|\frac{1}{\frac{1}{2}|p|^2+i\mu}\mathcal{F}(f)(p)\right|^2\,\mathrm{d}p &= \int_{\mathbb{R}^d}\frac{1}{|\frac{1}{2}|p|^2+i\mu|^2}|\mathcal{F}(f)(p)|^2\,\mathrm{d}p\\ &= \int_{\mathbb{R}^d}\frac{1}{\mu^2+\frac{1}{4}|p|^4}|\mathcal{F}(f)(p)|^2\,\mathrm{d}p\\ &\leqslant \frac{1}{\mu^2}\int_{\mathbb{R}^d}|\mathcal{F}(f)(p)|^2\,\mathrm{d}p = \frac{1}{\mu^2}\int_{\mathbb{R}^d}|f(x)|^2\,\mathrm{d}x < \infty.\end{aligned}$$

Now we can just define $u := \mathcal{F}^{-1}(\frac{1}{\frac{1}{2}|\cdot|^2+i\mu}\mathcal{F}(f) \in L^2(\mathbb{R}^d;\mathbb{C}))$ and obtain the desired function.

Step 2. We show that $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$ and satisfies $-\frac{1}{2}\Delta u + \mu i u = f$.

It remains to show that $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$. Using that $\mathcal{F}(u)(p) = \frac{1}{\frac{1}{2}|p|^2+i\mu}\mathcal{F}(f)(p)$ for a.e. $p \in \mathbb{R}^d$ we may compute

$$|p|^2\mathcal{F}(u)(p) = \frac{|p|^2}{\frac{1}{2}|p|^2+i\mu}\mathcal{F}(f)(p) \qquad \text{for a.e. } p \in \mathbb{R}^d$$

and thus $p \mapsto |p|^2\mathcal{F}(u)(p)$ is a product of the bounded function $p \mapsto \frac{|p|^2}{\frac{1}{2}|p|^2+i\mu}$ and the L^2-function $\mathcal{F}(f)$. As a result, $|\cdot|^2\mathcal{F}(u)$ lies in $L^2(\mathbb{R}^d;\mathbb{C})$, i.e.

$$\int_{\mathbb{R}^d}|p|^4|\mathcal{F}(u)(p)|^2\,\mathrm{d}p < \infty.$$

Since also $u \in L^2(\mathbb{R}^d;\mathbb{C})$ we have $\int_{\mathbb{R}^d} 1\cdot|\mathcal{F}(u)(p)|^2\,\mathrm{d}p < \infty$ and thus conclude

$$\int_{\mathbb{R}^d}(1+|p|^4)|\mathcal{F}(u)(p)|^2\,\mathrm{d}p < \infty.$$

Notice also that for all $p \in \mathbb{R}^d$ we have

$$(1+|p|^2)^2 = 1+2|p|^2+|p|^4 \leqslant 1+2\frac{1+|p|^4}{2}+|p|^4 \leqslant 2(1+|p|^4).$$

For this reason we have

$$\int_{\mathbb{R}^d}(1+|p|^2)^2|\mathcal{F}(u)(p)|^2\,\mathrm{d}p < \infty$$

showing that $u \in W_2$ in the sense of Part II Definition 10.1. Proposition 10.2 of Part II shows that then $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$. The claim follows using the fact $-\frac{1}{2}\Delta u + \mu i u = f$ and (55) are equivalent under the condition that $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$.

[a] In particular, with the special case $\mu = 1$ we deduce self-adjointess of $-\frac{1}{2}\Delta$. We will only learn later why we have introduced an extra factor $\mu > 0$ here.

[b]This requires a quick check that for $u \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$ the Fourier transform also satisfies the derivative rules of Remark 2.2.8 (these formulae are so far only known for $u \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$) We leave this as an exercise, along the lines of the proof of the intermediate claim in Proposition 2.2.11.

3.2.2.1 Self-Adjointness of the Schrödinger operator Recall now that we are interested in the Schrödinger operator H, formally expressable as $H = -\frac{1}{2}\Delta + M_V$, using the notation of the previous two examples. The previous two examples show that both "summands" $-\frac{1}{2}\Delta$ as well as M_V are self-adjoint operators. But is the sum of two self-adjoint operators also self-adjoint? The answer is unfortunately: in general no (at least if they are unbounded in $L^2(\mathbb{R}^d;\mathbb{C})$)! In this paragraph we deal with this issue and formulate conditions which ensure the self-adjointness of the sum of the operators and as a result also of our Schrödinger operator. First we define the sum of two operators rigorously.

Definition 3.2.22 — Operator sum

Let $A : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $B : D(B) \to L^2(\mathbb{R}^d;\mathbb{C})$ be two operators. Then we define the *operator sum*

$$A + B : D(A) \cap D(B) \to L^2(\mathbb{R}^d;\mathbb{C}), \qquad (A+B)\varphi := A\varphi + B\varphi.$$

(We sometimes also write $D(A+B) = D(A) \cap D(B)$)

The self-adjointness of the sum of two operators can be detected by the famous *Kato-Rellich* theorem.

Theorem 3.2.23 — Kato-Rellich

Suppose that $A : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $B : D(B) \to L^2(\mathbb{R}^d;\mathbb{C})$ are two symmetric operators. Further suppose that

(i) $D(A) \subseteq D(B)$

(ii) There exists some $a \in [0,1)$ and $c > 0$ such that $\|B\varphi\|_{L^2} \leqslant a\|A\varphi\|_{L^2} + c\|\varphi\|_{L^2}$ for all $\varphi \in D(A)$.

(iii) For all $\mu > 0$ the operators $A + \mu i\mathrm{Id} : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $A - \mu i\mathrm{Id} : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ are surjective[a]

Then $A + B : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint.

[a]In particular, (see Proposition 3.2.18 and look at the special case $\mu = 1$), A is self adjoint. If we had shown the converse in 3.2.18 we could replace this by the requirement that A is self-adjoint.

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Proof. For the sake of simplicity of notation we will in this proof write $A + \mu i$ instead of $A + \mu i\mathrm{Id}$. We will show that there exists $\mu_0 > 0$ such that $A + B \pm i\mu_0 : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ is surjective $(*)$, in particular also $\frac{A+B}{\mu} \pm i : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ are surjective. If we have this, then the self-adjointness criterion (Proposition 3.2.18) yield that $\frac{1}{\mu_0}(A+B) : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint. One readily checks as an easy exercise that then also $A+B$ is self-adjoint. Before we start the proof, let us mention that one can show along the lines of 3.2.20 that for each $\mu > 0$ the operators $A \pm i\mu : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ are injective. Due to this and prerequisite (iii) they are bijective and we may form $(A \pm i\mu)^{-1} : L^2(\mathbb{R}^d;\mathbb{C}) \to D(A)$. Let us now turn to the proof of $(*)$ For $\mu > 0$ and $\varphi \in D(A)$ we form

$$(A+B+i\mu)\varphi = (A+i\mu+B)(A+i\mu)^{-1}(A+i\mu)\varphi = (\mathrm{Id} + B(A+i\mu)^{-1})(A+i\mu)\varphi. \tag{56}$$

Now, prerequisite (iii) yields that $A + i\mu$ is surjective. Hence it suffices to show that $\mathrm{Id} + B(A+i\mu)^{-1} : L^2(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is surjective. To this end we use the Neumann series (Lemma 3.2.24). To check the prerequisites of the Neumann series we have to check that

$$\|B(A+i\mu)^{-1}\| := \sup_{f \in L^2(\mathbb{R}^d;\mathbb{C}), \|f\|=1} \|B(A+i\mu)^{-1}f\|_{L^2} < 1.$$

To check this let $f \in L^2(\mathbb{R}^d;\mathbb{C})$ be such that $\|f\|_{L^2} = 1$. Then prerequisite (ii) yields that for some $a \in [0,1)$ and $c > 0$ we have

$$\|B(A+i\mu)^{-1}f\|_{L^2} \leqslant a\|A(A+i\mu)^{-1}f\|_{L^2} + c\|(A+i\mu)^{-1}f\|_{L^2} \tag{57}$$

To draw further conclusions from the estimate we need an intermediate claim

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Intermediate claim. For each $\varphi \in D(A)$ we have $\|(A+i\mu)\varphi\|_{L^2}^2 = \|A\varphi\|_{L^2}^2 + \mu^2\|\varphi\|_{L^2}^2$.

To prove this we expand the scalar product and write

$$\|(A+i\mu)\varphi\|_{L^2}^2 = \langle A\varphi + i\mu\varphi, A\varphi + i\mu\varphi\rangle = \|A\varphi\|_{L^2}^2 + 2\mathrm{Re}\langle A\varphi, i\mu\varphi\rangle + \|i\mu\varphi\|_{L^2}^2.$$

The last term clearly equals $\mu^2\|\varphi\|_{L^2}^2$. Moreover we have

$$\mathrm{Re}\langle A\varphi, i\mu\varphi\rangle = \mathrm{Re}(-i\mu\langle A\varphi, \varphi\rangle) = 0,$$

since $\langle A\varphi, \varphi\rangle = \langle \varphi, A\varphi\rangle = \overline{\langle A\varphi, \varphi\rangle}$ and thus $\langle A\varphi, \varphi\rangle \in \mathbb{R}$, cf. Remark 2.1.8.

The intermediate claim (applied to $\varphi = (A+i\mu)^{-1}f \in D(A)$) implies

$$\|A(A+i\mu)^{-1}f\|_{L^2} = \|A\varphi\|_{L^2} \leqslant \sqrt{\|A\varphi\|_{L^2}^2 + \mu^2\|\varphi\|_{L^2}^2} = \sqrt{\|(A+i\mu)\varphi\|_{L^2}^2} = \|f\|_{L^2}.$$

and

$$\mu\|(A+i\mu)^{-1}f\|_{L^2} = \mu\|\varphi\|_{L^2} \leqslant \sqrt{\|A\varphi\|_{L^2}^2 + \mu^2\|\varphi\|_{L^2}^2} = \sqrt{\|(A+i\mu)\varphi\|_{L^2}^2} = \|f\|_{L^2}.$$

so that $\|A(A+i\mu)^{-1}f\|_{L^2} \leqslant \|f\|_{L^2}$ and $\|(A+i\mu)^{-1}f\|_{L^2} \leqslant \frac{1}{\mu}\|f\|_{L^2}$. Using this in (57) we find for $f \in L^2(\mathbb{R}^d;\mathbb{C})$ with $\|f\|_{L^2} = 1$

$$\|B(A+i\mu)^{-1}f\|_{L^2} \leqslant a\|f\|_{L^2} + \frac{c}{\mu}\|f\|_{L^2} = a + \frac{c}{\mu}.$$

Choosing $\mu_0 > \frac{c}{1-a}$ we obtain from this that

$$\|B(A+i\mu_0)\| < 1.$$

The Neumann series (Lemma 3.2.24) shows invertibility of $\mathrm{Id} + B(A+i\mu_0)$ and hence (56) (in the special case of $\mu = \mu_0$) yields surjectivity of $A+B+i\mu_0$. As described in the beginning of this proof, self adjointness of $A+B$ follows.

We have used the following result from functional analysis

Lemma 3.2.24 — Neumann Series

Let X be a Banach space and $T : X \to X$ be such that $\|T\| < 1$ (Recall that $\|T\| := \sup\limits_{x\in X:\|x\|_X=1} \|Tx\|_X$). Then $\mathrm{Id} + T : X \to X$ is invertible and

$$(\mathrm{Id}+T)^{-1} = \sum_{k=0}^{\infty} T^k.$$

We will next apply the Kato-Rellich theorem with $A = -\frac{1}{2}\Delta$ and $B = M_V$ (for some suitably chosen V) An easy example is given by bounded potentials $V \in L^\infty(\mathbb{R}^d;\mathbb{R})$.

Example 3.2.25

Let $V \in L^\infty(\mathbb{R}^d;\mathbb{R})$. In particular $D(M_V) = \{f \in L^2(\mathbb{R}^d;\mathbb{C}) : Vf \in L^2(\mathbb{R}^d;\mathbb{C})\} = L^2(\mathbb{R}^d;\mathbb{C})$.

Claim. $H = -\frac{1}{2}\Delta + M_V : W^{2,2}(\mathbb{R}^d;\mathbb{C}) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint.

Proof. We apply the Rellich-Kato-Theorem 3.2.23 with $A = -\frac{1}{2}\Delta$ and $B = M_V$. (i) is clear since $W^{2,2}(\mathbb{R}^d;\mathbb{C}) \subset L^2(\mathbb{R}^d;\mathbb{C})$. (iii) follows directly from Remark 3.2.21. Now we prove (ii) (actually with $a = 0$). To this end we compute for $\varphi \in L^2(\mathbb{R}^d;\mathbb{C}$

$$\|M_V\varphi\|_{L^2}^2 = \int_{\mathbb{R}^d} |V(x)\varphi(x)|^2 \,\mathrm{d}x = \int_{\mathbb{R}^d} \|V\|_{L^\infty}^2 |\varphi(x)|^2 \,\mathrm{d}x = \|V\|_{L^\infty}^2 \|\varphi\|_{L^2}^2.$$

As a result $\|M_V\varphi\|_{L^2} \leqslant \|V\|_{L^\infty}\|\varphi\|_{L^2}$, i.e. (ii) holds with $a = 0$ and $c = \|V\|_{L^\infty}$. The Kato-Rellich Theorem applies and self-adjointness is ensured.

While it is nice to have a first condition on V so that the Schrödinger operator is self-adjoint, this condition is not physically meaningful. Indeed, let us illustrate this with a very basic example from physics. If our particle is an electron in $\mathbb{R}^3$ which is part of an atom centered at the origin, we must (since the nucleus has positive charge) look at the *Coulomb potential*

$$V : \mathbb{R}^3 \backslash \{0\} \to \mathbb{R}, \qquad V(x) = \frac{1}{4\pi\varepsilon_0} \frac{1}{|x|}.$$

(Notice that at the value $x = 0$ we have to assign some other value to V whose precise choice does not matter for the discusson). This potential does clearly not lie in $L^\infty(\mathbb{R}^3; \mathbb{R})$. For this reason we need a better result than the one in Example 3.2.25.

Proposition 3.2.26 — Self-Adjointness of the Schrödinger operator

Let $d = 3$. Let $V : \mathbb{R}^3 \to \mathbb{R}$ be such that $V = V_1 + V_2$ for some $V_1 \in L^2(\mathbb{R}^3; \mathbb{R})$ and $V_2 \in L^\infty(\mathbb{R}^3; \mathbb{R})$. Then $H = -\frac{1}{2}\Delta + M_V : W^{2,2}(\mathbb{R}^3; \mathbb{C}) \to L^2(\mathbb{R}^3; \mathbb{C})$ is self-adjoint.

We will in the sequel often write $V \in L^2(\mathbb{R}^3; \mathbb{R}) + L^\infty(\mathbb{R}^3; \mathbb{R})$ to express that $V = V_1 + V_2$ for $V_1 \in L^2(\mathbb{R}^3; \mathbb{R})$ and $V_2 \in L^\infty(\mathbb{R}^3; \mathbb{R})$.

Proof (of Proposition 3.2.26). We again apply the Rellich-Kato-Theorem 3.2.23 with $A = -\frac{1}{2}\Delta : W^{2,2}(\mathbb{R}^3; \mathbb{C}) \to L^2(\mathbb{R}^3; \mathbb{C})$ and $B = M_V : D(M_V) \to L^2(\mathbb{R}^3; \mathbb{C})$, where as always

$$D(M_V) = \{f \in L^2(\mathbb{R}^3; \mathbb{C}) : Vf \in L^2(\mathbb{R}^3; \mathbb{C})\}.$$

We now check Condition (i),(ii),(iii) in Theorem 3.2.23. Condition (iii) again follows directly from Example 3.2.21. Condition (i) is now nontrivial but it will fall out of the verification of Condition (ii). More precisely we show the following

Main Claim. There exists $a \in [0, 1)$ and $c > 0$ such that for all $\varphi \in W^{2,2}(\mathbb{R}^3; \mathbb{C})$ we have $\|V\varphi\|_{L^2} \leqslant a\|A\varphi\|_{L^2} + c\|\varphi\|_{L^2}$ $(*)$

This shows that for each $\varphi \in D(A) = W^{2,2}(\mathbb{R}^3; \mathbb{C})$ we have $V\varphi \in L^2(\mathbb{R}^3; \mathbb{C})$ and thus $\varphi \in D(M_V)$, which settles (i). Once this is observed, the estimate $(*)$ boils down to Condition (ii). Hence we turn to the proof of $(*)$. First recall from Example 3.2.25 that for each $\varphi \in D(M_V) \subset L^2(\mathbb{R}^3; \mathbb{C})$ we have

$$\|V_2\varphi\|_{L^2} \leqslant \|V_2\|_{L^\infty}\|\varphi\|_{L^2} \tag{58}$$

Now we have to estimate $\|V_1\varphi\|_{L^2}$. To this end we first estimate for $\varphi \in D(M_V)$

$$\|V_1\varphi\|_{L^2} \leqslant \|V_1\|_{L^2}\|\varphi\|_{L^\infty}, \tag{59}$$

(where we mean $\|\varphi\|_{L^\infty} = \infty$ if $\varphi \notin L^\infty$).

Intermediate claim. Let $\varepsilon > 0$ be arbitrary. For $\varphi \in W^{2,2}(\mathbb{R}^3; \mathbb{C}$ define $\hat{\varphi} := \mathcal{F}(\varphi)$. Then $\hat{\varphi} \in L^1(\mathbb{R}^3; \mathbb{C})$ and $\|\hat{\varphi}\|_{L^1} \leqslant \varepsilon\|A\varphi\|_{L^2} + d_\varepsilon\|\varphi\|_{L^2}$ for some $d_\varepsilon > 0$ (independent of φ).

To prove this we first write

$$\|\hat{\varphi}\|_{L^1} = \int_{\mathbb{R}^3} |\hat{\varphi}(x)| \,\mathrm{d}x = \int_{\mathbb{R}^3} \frac{1}{1+|x|^2}(1+|x|^2)|\hat{\varphi}(x)| \,\mathrm{d}x$$
$$\leqslant \sqrt{\int_{\mathbb{R}^3} \frac{1}{(1+|x|^2)^2} \,\mathrm{d}x}\sqrt{\int_{\mathbb{R}^3} (1+|x|^2)^2|\hat{\varphi}(x)|^2 \,\mathrm{d}x} \tag{60}$$

The last factor yields

$$\sqrt{\int_{\mathbb{R}^3} (1+|x|^2)^2|\hat{\varphi}(x)|^2 \,\mathrm{d}x} = \|(1+|\cdot|^2)\hat{\varphi}\|_{L^2} = \|\hat{\varphi}+|\cdot|^2\hat{\varphi}\|_{L^2} \leqslant \|\hat{\varphi}\|_{L^2} + \||\cdot|^2\hat{\varphi}\|_{L^2}$$
$$= \|\varphi\|_{L^2} + \|\Delta\varphi\|_{L^2} = \|\varphi\|_{L^2} + 2\|A\varphi\|_{L^2}$$

The first factor in (60) is a finite constant since radial integration[a] yields

$$\int_{\mathbb{R}^3} \frac{1}{(1+|x|^2)^2} \,\mathrm{d}x = \int_0^\infty \frac{4\pi r^2}{(1+r^2)^2} \,\mathrm{d}r = \int_0^1 \frac{4\pi r^2}{(1+r^2)^2} \,\mathrm{d}r + \int_1^\infty \frac{4\pi r^2}{(1+r^2)^2} \,\mathrm{d}r$$
$$\leqslant \int_0^1 \frac{4\pi\cdot 1}{(1+0)^2} \,\mathrm{d}r + \int_1^\infty \frac{4\pi r^2}{(0+r^2)^2} \,\mathrm{d}r$$
$$= 4\pi + 4\pi\int_1^\infty \frac{1}{r^2} \,\mathrm{d}r = 4\pi + 4\pi\left[-\frac{1}{r}\right]_1^\infty = 8\pi.$$

Using this (60) yields

$$\|\hat{\varphi}\|_{L^1} \leqslant \sqrt{8\pi}(\|\varphi\|_{L^2} + 2\|A\varphi\|_{L^2}).$$

This is not quite what we wanted since the intermediate claim demands a small prefactor in front of $\|A\varphi\|_{L^2}$. To refine the estimate define for $r>0$ the function $\hat{\varphi}_r := r^3\varphi(r\cdot)$ and observe that $\|\hat{\varphi}\|_{L^1} = \|\hat{\varphi}_r\|_{L^1}$, as is easily seen with the transformation formula[b]. Repeating now the steps in (60) we find that

$$\|\hat{\varphi}_r\|_{L^1} \leqslant \sqrt{8\pi}\|(1+|\cdot|^2)\hat{\varphi}_r\|_{L^2} \leqslant \sqrt{8\pi}\|\hat{\varphi}_r\|_{L^2} + \sqrt{8\pi}\||\cdot|^2\hat{\varphi}_r\|_{L^2} \tag{61}$$

Now we compute

$$\|\hat{\varphi}_r\|_{L^2}^2 = \int_{\mathbb{R}^3} r^6|\hat{\varphi}(rx)|^2 \,\mathrm{d}x = r^3\int_{\mathbb{R}^3} |\hat{\varphi}(y)|^2 \,\mathrm{d}y = r^3\|\hat{\varphi}\|_{L^2}^2,$$

so that $\|\hat{\varphi}_r\|_{L^2} = r^{\frac{3}{2}}\|\hat{\varphi}\|_{L^2}$. Moreover

$$\||\cdot|^2\hat{\varphi}_r\|_{L^2}^2 = \int_{\mathbb{R}^3} |x|^4r^6|\hat{\varphi}(rx)|^2 \,\mathrm{d}x = r^2\int_{\mathbb{R}^3} |rx|^4|\hat{\varphi}(rx)|^2 \,\mathrm{d}x = r^{-1}\int_{\mathbb{R}^3} |y|^4|\hat{\varphi}(y)|^2 \,\mathrm{d}y,$$

soe that $\||\cdot|^2\hat{\varphi}_r\|_{L^2} = r^{-\frac{1}{2}}\||\cdot|^2\hat{\varphi}\|_{L^2}$. Using these findings in (61) we obtain

$$\begin{aligned}\|\hat{\varphi}\|_{L^1} = \|\hat{\varphi}_r\|_{L^1} &\leqslant \sqrt{8\pi}(r^{-\frac{1}{2}}\||\cdot|^2\hat{\varphi}\|_{L^2} + r^{\frac{3}{2}}\|\hat{\varphi}\|_{L^2}) \\ &= \sqrt{8\pi}(r^{-\frac{1}{2}}\|\Delta\varphi\|_{L^2} + r^{\frac{3}{2}}\|\varphi\|_{L^2}) = \sqrt{8\pi}(2r^{-\frac{1}{2}}\|A\varphi\|_{L^2} + r^{\frac{3}{2}}\|\varphi\|_{L^2}).\end{aligned}$$

Now we may choose $r_0 = r_0(\varepsilon) > 0$ such that $2\sqrt{8\pi}r_0^{-\frac{1}{2}} = \varepsilon$. Defining $d_\varepsilon := \sqrt{8\pi}r_0^{\frac{3}{2}}$ we obtain

$$\|\hat{\varphi}\|_{L^1} \leqslant \varepsilon\|A\varphi\|_{L^2} + d_\varepsilon\|\varphi\|_{L^2},$$

as claimed.

Next we employ Lemma 3.2.27 (see also Theorem 6.15 in Part II) and the intermediate claim to obtain for fixed $\varepsilon > 0$

$$\|\varphi\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\|\mathcal{F}(\varphi)\|_{L^1} = \frac{1}{(2\pi)^{\frac{d}{2}}}\left(\varepsilon\|A\varphi\|_{L^2} + d_\varepsilon\|\varphi\|_{L^2}\right).$$

This and (59) and (58) yield

$$\begin{aligned}\|V\varphi\|_{L^2} &\leqslant \|V_1\varphi + V_2\varphi\|_{L^2} \leqslant \|V_1\varphi\|_{L^2} + \|V_2\varphi\|_{L^2} \leqslant \|V_1\|_{L^2}\|\varphi\|_{L^\infty} + \|V_2\|_{L^\infty}\|\varphi\|_{L^2} \\ &= \frac{\|V_1\|_{L^2}}{(2\pi)^{\frac{d}{2}}}\left(\varepsilon\|A\varphi\|_{L^2} + d_\varepsilon\|\varphi\|_{L^2}\right) + \|V_2\|_{L^\infty}\|\varphi\|_{L^2} \\ &= \varepsilon\frac{\|V_1\|_{L^2}}{(2\pi)^{\frac{d}{2}}}\|A\varphi\|_{L^2} + \left(\frac{\|V_1\|_{L^2}}{(2\pi)^{\frac{d}{2}}}d_\varepsilon + \|V_2\|_{L^\infty}\right)\|\varphi\|_{L^2}.\end{aligned}$$

Choosing $\varepsilon_0 := \frac{1}{2}\left(\frac{\|V_1\|_{L^2}}{(2\pi)^{\frac{d}{2}}} + 1\right)^{-1}$ we obtain some $c := \left(\frac{\|V_1\|_{L^2}}{(2\pi)^{\frac{d}{2}}}d_{\varepsilon_0} + \|V_2\|_{L^\infty}\right) > 0$ such that for all $\varphi \in W^{2,2}(\mathbb{R}^d;\mathbb{C})$ we have

$$\|V\varphi\|_{L^2} \leqslant \tfrac{1}{2}\|A\varphi\|_{L^2} + c\|\varphi\|_{L^2}.$$

The mein claim is shown and as discussed above our assertion follows.

[a] That is a substitution $(x, y, z) = (r\cos\varphi\cos\theta, r\sin\varphi\cos\theta, r\sin\theta)$, where $r \in (0,\infty)$, $\varphi \in (0, 2\pi), \theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$

[b] Indeed, the substitution $y = rx$ yields $\|\hat{\varphi}_r\|_{L^1} = \int_{\mathbb{R}^3} r^3|\hat{\varphi}(rx)|\,\mathrm{d}x = \int_{\mathbb{R}^3}|\hat{\varphi}(y)|\,\mathrm{d}y = \|\hat{\varphi}\|_{L^1}$.

The proof again relied on an auxiliary lemma. For the first part of this lemma see also Theorem 6.15 in Part II.

Lemma 3.2.27

(i) Let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$. Then $\mathcal{F}(\varphi) \in L^\infty(\mathbb{R}^d;\mathbb{C})$ and

$$\|\mathcal{F}(\varphi)\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\|\varphi\|_{L^1}$$

(ii) Let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ be such that $\mathcal{F}(\varphi) \in L^1(\mathbb{R}^d;\mathbb{C})$. Then $\varphi \in L^\infty(\mathbb{R}^d;\mathbb{C})$ and

$$\|\varphi\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\|\mathcal{F}(\varphi)\|_{L^1}$$

Proof. Ad (i). Let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$. As shown in the intermediate claim of Theorem 3.1.13 one can find $(\varphi_n)_{n\in\mathbb{N}} \subseteq \mathcal{S}(\mathbb{R}^d;\mathbb{C})$ such that $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$ and $\varphi_n \xrightarrow[L^1(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$. Note that for each $x \in \mathbb{R}^d$ we have

$$\mathcal{F}(\varphi_n)(x) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} \varphi_n(y)e^{ixy}\,\mathrm{d}y$$

This implies that for each $x \in \mathbb{R}^d$ we have

$$|\mathcal{F}(\varphi_n)(x)| = \left|\frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} \varphi_n(y)e^{-ixy}\,\mathrm{d}y\right| \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} |\varphi_n(y)|\,\mathrm{d}y = \frac{1}{(2\pi)^{\frac{d}{2}}}\|\varphi_n\|_{L^1}. \tag{62}$$

Now, since $(\varphi_n)_{n\in\mathbb{N}}$ converges in $L^2(\mathbb{R}^d;\mathbb{C})$ to φ we obtain that $(\mathcal{F}(\varphi_n))_{n\in\mathbb{N}}$ converges in $L^2(\mathbb{R}^d;\mathbb{C})$ to $\mathcal{F}(\varphi)$. For this reason we can use Proposition 2.3.17 in ↑ `Analysis III Lecture Notes` to extract a subsequence $(\mathcal{F}(\varphi_{\ell_n}))_{n\in\mathbb{N}}$ that converges pointwise a.e. to $\mathcal{F}(\varphi)$. As a result we obtain for a.e. $x \in \mathbb{R}^d$

$$|\mathcal{F}(\varphi)(x)| = \lim_{n\to\infty}|\mathcal{F}(\varphi_{\ell_n})(x)| \underset{(62)}{\leqslant} \limsup_{n\to\infty}\frac{1}{(2\pi)^{\frac{d}{2}}}\|\varphi_{\ell_n}\|_{L^1} = \frac{1}{(2\pi)^{\frac{d}{2}}}\|\varphi\|_{L^1}$$

where we have used in the last step that $\varphi_n \xrightarrow[L^1(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$. This implies

$$\|\mathcal{F}(\varphi)\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\|\varphi\|_{L^1}.$$

Ad (ii). Notice first that $\mathcal{F}(\varphi) \in L^2(\mathbb{R}^d;\mathbb{C}) \cap L^1(\mathbb{R}^d;\mathbb{C})$ and hence (i) yields $\mathcal{F}(\mathcal{F}(\varphi)) \in L^\infty$ and

$$\|\mathcal{F}(\mathcal{F}(\varphi))\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\|\mathcal{F}(\varphi)\|_{L^1}. \tag{63}$$

Now observe that $\mathcal{F}(\mathcal{F}(\varphi)) = \varphi(-(\cdot))$ for any $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. Indeed: We show the claim first for $\varphi \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. In this case we have for $x \in \mathbb{R}^d$

$$\mathcal{F}(\mathcal{F}(\varphi))(x) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} \mathcal{F}(\varphi)(y)e^{-ixy}\,\mathrm{d}y$$

$$= \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \mathcal{F}(\varphi)(y) e^{i(-x)y} \, \mathrm{d}y = \mathcal{F}^{-1}(\mathcal{F}(\varphi)(-x) = \varphi(-x),$$

which implies the claim for functions in $\mathcal{S}(\mathbb{R}^d; \mathbb{C})$ The claim can be extended to L^2-functions by approximation[a]. Combining this with (63) we now have $\varphi(-(\cdot)) = \mathcal{F}(\mathcal{F}(\varphi)) \in L^\infty(\mathbb{R}^d; \mathbb{C})$ and

$$\|\varphi(-(\cdot))\|_{L^\infty} = \|\mathcal{F}(\mathcal{F}(\varphi))\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}} \|\mathcal{F}(\varphi)\|_{L^1}.$$

One is readily convinced that $\|\varphi\|_{L^\infty} = \|\varphi(-(\cdot))\|_{L^\infty}$. For this reason we infer that $\varphi \in L^\infty(\mathbb{R}^d; \mathbb{C})$ and

$$\|\varphi\|_{L^\infty} \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}} \|\mathcal{F}(\varphi)\|_{L^1}.$$

The claim follows.

[a] Indeed, if we choose $(\eta_n)_{n\in\mathbb{N}} \subseteq \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ such that $\eta_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$ we conclude $\mathcal{F}(\mathcal{F}(\eta_n)) \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \mathcal{F}(\mathcal{F}(\varphi))$ (by unitariness of the Fourier transform). Moreover one readily checks that $\eta_n(-(\cdot)) \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi(-(\cdot))$. Based on these observations we compute

$$\mathcal{F}(\mathcal{F}(\varphi)) = \operatorname*{LIM}_{n\to\infty} \mathcal{F}(\mathcal{F}(\eta_n)) = \operatorname*{LIM}_{n\to\infty} \eta_n(-(\cdot)) = \varphi(-(\cdot)).$$

To convince you that the prerequisites on V in Proposition 3.2.26 are suitable for the applications we convince you that the Coulomb potential satisfies the estimates given there

Example 3.2.28

Let

$$V : \mathbb{R}^3 \to \mathbb{R}, \quad V(x) := \begin{cases} \frac{1}{4\pi\varepsilon_0} \frac{1}{|x|} & x \in \mathbb{R}^3 \backslash \{0\} \\ 0 & x = 0. \end{cases}$$

Claim. $H = -\frac{1}{2}\Delta + M_V : W^{2,2}(\mathbb{R}^d; \mathbb{C}) \to L^2(\mathbb{R}^d; \mathbb{C})$ is self-adjoint.

Proof. According to the previous proposition we just have to write $V = V_1 + V_2$ as a sum of $V_1 \in L^2(\mathbb{R}^3; \mathbb{C})$ and $V_2 \in L^\infty(\mathbb{R}^3; \mathbb{C})$. We will now convince ourselves that

$$V_1 := V\chi_{B_1(0)}, \qquad V_2 := V\chi_{\mathbb{R}^3 \backslash B_1(0)}$$

does the job.

Clearly, $V_2 \in L^\infty(\mathbb{R}^3; \mathbb{C})$ as for all $x \in \mathbb{R}^3 \backslash B_1(0)$ we have $|x| \geqslant 1$ and thus

$$V(x) = \frac{1}{4\pi\varepsilon_0 |x|} \leqslant \frac{1}{4\pi\varepsilon_0}.$$

This yields $\|V_2\|_{L^\infty} \leqslant \frac{1}{4\pi\varepsilon_0} < \infty$.

To show that $V_1 \in L^2(\mathbb{R}^3; \mathbb{C})$ we compute

$$\int_{B_1(0)} |V(x)|^2 \;\mathrm{d}x = \frac{1}{(4\pi\varepsilon_0)^2} \int_{B_1(0)} \frac{1}{|x|^2} \,\mathrm{d}x$$

Using again radial integration[a] in $\mathbb{R}^3$ we find

$$\int_{B_1(0)} \frac{1}{|x|^2} \,\mathrm{d}x = \int_0^1 \frac{4\pi r^2}{r^2} \,\mathrm{d}r = 4\pi < \infty.$$

This yields

$$\int_{B_1(0)} |V(x)|^2 \;\mathrm{d}x < \infty$$

and hence the claim.

[a] That is a substitution $(x, y, z) = (r\cos\varphi\cos\theta, r\sin\varphi\cos\theta, r\sin\theta)$, where $r \in (0, 1)$, $\varphi \in (0, 2\pi), \theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$

4 Trotter's Product Formula and Path Integrals

We have finally understood what a solution of the Schrödinger equation is (Axiom 3.0.1). Then means define a notion of solutions to the Schrödinger equation, even for nonsmooth initial data $\psi_0 \in L^2(\mathbb{R}^3;\mathbb{C})$. We have also seen that one needs conditions on the potential to formulate it rigorously, e.g. $V \in L^2(\mathbb{R}^3;\mathbb{R}) + L^\infty(\mathbb{R}^3;\mathbb{R})$ (which we will assume throughout this chapter).

Having a formulation of a problem is nice, but in the end we want to *compute solutions* – because this is also what physicists would expect from a mathematical theory (the answer "yes the Schrödinger equation is well-posed" is probably not very satisfactory...).

Hence we will discuss how the solution can be computed by means of *path integrals* (a notion that lacks a little bit a rigorous definition, but we will be able to write down what it a path integral means mathematically).

Let $V \in L^2(\mathbb{R}^3;\mathbb{R}) + L^\infty(\mathbb{R}^3;\mathbb{R})$. We know from Proposition 3.2.26 that $H = -\frac{1}{2}\Delta + M_V : W^{2,2}(\mathbb{R}^3,\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C})$ is self-adjoint. In particular, Stone's Theorem (Theorem 3.2.13) shows that there exists a unitary group $(e^{-itH})_{t\in\mathbb{R}} = (e^{-it(-\frac{1}{2}\Delta + M_V)})_{t\in\mathbb{R}}$. Now we would like to find an explicit formula to compute this group. We already know how the SCU-group associated to the summands $-\frac{1}{2}\Delta$ and M_V look like. Indeed, recall from the discussion below Example 3.2.15 that for each $\varphi \in L^2(\mathbb{R}^3;\mathbb{C})$ we have

$$(e^{-itM_V}\varphi)(x) = e^{-itV(x)}\varphi(x) \qquad \text{a.e. } x \in \mathbb{R}^3 \tag{64}$$

Moreover, recall from (41) and the discussion before as well as Proposition 3.2.17 that for all $\varphi \in L^2(\mathbb{R}^3;\mathbb{C})$ we have (if $t \neq 0$)

$$(e^{-it(-\frac{1}{2}\Delta)}\varphi)(x) = \frac{1}{(2\pi i t)^{\frac{3}{2}}} \tilde{\int_{\mathbb{R}^d}} e^{i\frac{|x-y|^2}{2t}}\varphi(y)\,\mathrm{d}y \qquad \text{a.e. } x \in \mathbb{R}^3 \tag{65}$$

That means, for each summand we already know the generated SCU-group. One naive approach would now be to hope that the functional equality of the exponential function applies and we somehow have the following

$$\textbf{Hope (turns out to be wrong):} \quad e^{-itH} = e^{-it(-\frac{1}{2}\Delta + M_V)} = e^{-it(-\frac{1}{2}\Delta)} \circ e^{-itM_V}. \tag{66}$$

But this is false. To understand why this is false and how to correct it, we start very simple with some observations in finite dimensions. Generalizing these to infinite dimension will already yield an approximation formula for e^{-itH}.

4.0.1 The finite dimensional case

We would now like to investigate (66) further. And to be simple we start with a finite-dimensional consideration

Definition 4.0.1 — Unitary Matrix Exponential

Let $A \in \mathbb{C}^{n\times n}$ be a matrix and $t \in \mathbb{R}$. We define the *unitary matrix exponential*

$$e^{-itA} := \lim_{m\to\infty} \sum_{k=0}^{m} \frac{(-itA)^k}{k!} \in \mathbb{C}^{n\times n}, \tag{67}$$

where $A^0 := I_{n\times n}$ is the identitiy matrix and the limit can be understood with respect to any norm in $\mathbb{C}^{n\times n}$ (which one is taken is irrelevant as two norms on $\mathbb{C}^{n\times n}$ are equivalent).

To check that this is well-defined we have to ensure that the series in (67) converges for all $t \in \mathbb{R}$ and $A \in \mathbb{C}^{n\times n}$. This is seen as follows. First of all recall that one can find a norm $\|\cdot\|_{\mathbb{C}^{n\times n}}$ on $\mathbb{C}^{n\times n}$ such that for $A, B \in \mathbb{C}^{n\times n}$ we have[2]

$$\|A \cdot B\|_{\mathbb{C}^{n\times n}} \leqslant \|A\|_{\mathbb{C}^{n\times n}} \cdot \|B\|_{\mathbb{C}^{n\times n}}. \tag{68}$$

In particular, for $k \in \mathbb{N}$ we have $\|A^k\|_{\mathbb{C}^{n\times n}} = \|A\|^k_{\mathbb{C}^{n\times n}}$. As a result we compute for each $t \in \mathbb{R}$ that

$$\sum_{k=0}^{\infty} \left\| \frac{(-itA)^k}{k!} \right\|_{\mathbb{C}^{n\times n}} \leqslant \sum_{k=0}^{\infty} \frac{|t|^k \|A\|^k_{\mathbb{C}^{n\times n}}}{k!} = e^{|t|\,\|A\|_{\mathbb{C}^{n\times n}}} < \infty.$$

In particular, $\sum\limits_{k=0}^{\infty} \frac{(-itA)^k}{k!}$ converges absolutely and hence also converges[3]. Moreover this and the triangle inequality reveals that

$$\left\|e^{-itA}\right\|_{\mathbb{C}^{n\times n}} = \left\| \sum_{k=0}^{\infty} \frac{(-itA)^k}{k!} \right\|_{\mathbb{C}^{n\times n}} \leqslant e^{|t|\,\|A\|_{\mathbb{C}^{n\times n}}} \tag{69}$$

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To check the plausibility of (66), we would like to investigate whether for two matrices $A, B \in \mathbb{C}^{n\times n}$ one has $e^{-it(A+B)} = e^{-itA}e^{-itB}$. For $n = 1$ this is true, since 1×1-matrices are just complex numbers and then we just have the standard exponential function in $\mathbb{C}$. For $t = 0$ the relation is also always true regardless of the value of n as one readily checks with (67) that $e^0 = I_{n\times n}$. But already for $n = 2$ and any $t \neq 0$ this relation can be false.

Example 4.0.2

Suppose that $A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$.

[2] If you have attended functional analysis, you would probably be inclined to take the operator norm. What however also does the job is the *Hilbert-Schmidt-Norm*: For $A = (a_{ij})_{i,j=1,\dots,n}$ the Hilbert-Schmidt norm is defined as

$$\|A\|_{\mathbb{C}^{n\times n}} := \sqrt{\sum_{i,j=1}^{n} |a_{ij}|^2}.$$

One is readily convinced that then $\|A \cdot B\|_{\mathbb{C}^{n\times n}} \leqslant \|A\|_{\mathbb{C}^{n\times n}}\|B\|_{\mathbb{C}^{n\times n}}$

[3] Here we used that in Banach spaces absolutely convergent series are also convergent. If you have seen that not in this generality you can probably easily prove it in $\mathbb{C}^n$ - the precise choice of the norm does not play a role in this special case as all norms are equivalent.

Claim. $e^{-it(A+B)} \neq e^{-itA}e^{-itB}$ for all $t \neq 0$.

Proof. First note that A is a diagonal matrix and hence for all $k \in \mathbb{N}_0$

$$A^k = \begin{pmatrix} 1^k & 0 \\ 0 & 0^k \end{pmatrix}$$

Therefore one has for all $t \in \mathbb{R}$

$$e^{-itA} = \lim_{m\to\infty} \sum_{k=0}^{m} \frac{1}{k!} \begin{pmatrix} (-it)^k & 0 \\ 0 & 0^k \end{pmatrix} = \begin{pmatrix} \sum_{k=0}^{\infty} \frac{(-it)^k}{k!} & 0 \\ 0 & \sum_{k=0}^{\infty} \frac{0^k}{k!} \end{pmatrix} = \begin{pmatrix} e^{-it} & 0 \\ 0 & 1 \end{pmatrix}$$

For B we compute

$$B^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad B^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad B^2 = B^3 = B^4 = \dots = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Hence for all $m \geqslant 2$ we have

$$\sum_{k=0}^{m} \frac{(-itB)^k}{k!} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & -it \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -it \\ 0 & 1 \end{pmatrix}$$

And thus

$$e^{-itB} = \begin{pmatrix} 1 & -it \\ 0 & 1 \end{pmatrix}$$

As a result we have

$$e^{-itA}e^{-itB} = \begin{pmatrix} e^{-it} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -it \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} e^{-it} & -ite^{-it} \\ 0 & 1 \end{pmatrix}. \tag{70}$$

Now define

$$C := A + B = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$$

One readily checks that $C^2 = C$. As a result one has $C^k = C$ for all $k \geqslant 1$ and thus for $m \geqslant 2$ one has

$$\sum_{k=0}^{m} \frac{(-itC)^k}{k!} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sum_{k=1}^{m} \frac{(-it)^k}{k!} C$$

Letting $m \to \infty$ we obtain

$$e^{-itC} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \left(\sum_{k=1}^{\infty} \frac{(-it)^k}{k!} \right) C = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + (e^{-it} - 1) \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} e^{-it} & e^{-it} - 1 \\ 0 & 1 \end{pmatrix}.$$

Now we compare this result to (70) and find that $e^{-itA}e^{-itB} = e^{-it(A+B)}$ iff $e^{-it}-1 = -ite^{-it}$. We claim that this is not true for any $t \neq 0$. Assume that it is true for some $t \neq 0$. We multiply by e^{it} and find that the expression is equivalent to

$$1 - e^{it} = -it$$

Taking real and imaginary part we find $1 - \cos(t) = 0$ and $\sin(t) = t$. As a result we find

$$1 = \cos^2(t) + \sin^2(t) = 1^2 + t^2 = 1 + t^2,$$

yielding $t = 0$, a contradiction.

There is however one special case where the relation in which $e^{-it(A+B)} = e^{-itA}e^{-itB}$ $\forall t \in \mathbb{R}$ holds true: Namely **if and only if** A and B *commute*.

Proposition 4.0.3

Let $A, B \in \mathbb{C}^{n\times n}$. Then the following are equivalent

- $AB = BA$
- For all $t \in \mathbb{R}$ we have
$$e^{-it(A+B)} = e^{-itA}e^{-itB}. \tag{71}$$

We will not show a proof of this result that since it is purely finite-dimensional and not of our interest. What is much more important is the

Bottom Line. In general the commutation relation (71) is not true.

Instead we formulate an approximation result for $e^{-it(A+B)}$, which will have a helpful generalization to infinite dimensions. The approximation result is inspired by the following observation: If $a \in \mathbb{C}$ is some number then for all $m \in \mathbb{N}$

$$e^{-ita} = (e^{-i\frac{t}{m}a})^m \tag{72}$$

In particular e^{-ita} can be written as a product of exponentials with small exponents. Since the commutation relation $e^{-it(A+B)} = e^{-itA}e^{-itB}$ is certainly true for $t = 0$, maybe it *almost valid* for small t. Bringing this idea and (72) we obtain the following approximation result

Theorem 4.0.4 — Lie's product formula

Let $A, B \in \mathbb{C}^{n\times n}$ be matrices. Then for all $t \in \mathbb{R}$ we have

$$e^{-it(A+B)} = \lim_{m\to\infty} \left(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B}\right)^m.$$

(Again the limit can be taken with respect to any matrix norm as all norms on $\mathbb{C}^{n\times n}$ are equivalent)

Proof. For this proof $\|\cdot\| : \mathbb{C}^{n\times n} \to \mathbb{R}$ will denote any matrix norm that satisfies the submultiplicativity estimate (68). Let $t \in \mathbb{R}$. Define for $m \in \mathbb{N}$ the matrices

$$S_m := e^{-i\frac{t}{m}(A+B)} \qquad T_m := e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B}.$$

Then we may use a telescopic sum to compute

$$S_m^m - T_m^m = \sum_{k=0}^{m-1} S_m^{k+1}T_m^{m-(k+1)} - S_m^k T_m^{m-k} = \sum_{k=0}^{m-1} S_m^k(S_m - T_m)T_m^{m-k-1}.$$

We now use the triangle inequality and the submultiplicativity to compute

$$\begin{aligned}
\|S_m^m - T_m^m\| &\leqslant \sum_{k=0}^{m-1} \|S_m^k(S_m - T_m)T_m^{m-k-1}\| \leqslant \sum_{k=0}^{m-1} \|S_m\|^k\|S_m - T_m\| \, \|T_m\|^{m-k-1} \\
&= \|S_m - T_m\| \sum_{k=0}^{m-1} \max\{\|S_m\|, \|T_m\|\}^k \max\{\|S_m\|, \|T_m\|\}^{m-k-1} \\
&= \|S_m - T_m\| \sum_{k=0}^{m-1} \max\{\|S_m\|, \|T_m\|\}^{m-1} = \|S_m - T_m\| m \max\{\|S_m\|, \|T_m\|\}^{m-1}
\end{aligned} \tag{73}$$

Now we estimate $\|S_m - T_m\|$. To this end we may write

$$S_m - T_m = e^{-i\frac{t}{m}(A+B)} - e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B} = \sum_{k=0}^{\infty} \frac{(-it(A+B))^k}{k!m^k} - \left(\sum_{k=0}^{\infty} \frac{(-itA)^k}{k!m^k}\right)\left(\sum_{k=0}^{\infty} \frac{(-itB)^k}{k!m^k}\right).$$

Now writing $O(\frac{1}{m^2})$ for terms whose product with m^2 is bounded (w.r.t. $\|\cdot\|$) as $m \to \infty$ we have

$$\begin{aligned}
S_m - T_m &= I + \frac{-it(A+B)}{m} + O(\tfrac{1}{m^2}) - (I + \frac{-itA}{m} + O(\tfrac{1}{m^2}))(I + \frac{-itB}{m} + O(\tfrac{1}{m^2})) \\
&= I + \frac{-it(A+B)}{m} + O(\tfrac{1}{m^2}) - I + \frac{-itA}{m}I - I\frac{-itB}{m} + O(\tfrac{1}{m^2}) \\
&= I - \frac{it(A+B)}{m} - I + \frac{itA}{m} + \frac{itB}{m} + O(\tfrac{1}{m^2}) = O(\tfrac{1}{m^2}).
\end{aligned}$$

Hence we obtain that $(m^2\|S_m - T_m\|)_{m\in\mathbb{N}}$ is bounded by some $C > 0$, i.e.

$$\|S_m - T_m\| \leqslant \frac{C}{m^2} \qquad \forall m \in \mathbb{N}$$

Using this in (73) we find

$$\|S_m^m - T_m^m\| \leqslant \frac{C}{m^2} m \max\{\|S_m\|, \|T_m\|\}^{m-1} = \frac{C}{m} \max\{\|S_m\|^{m-1}, \|T_m\|^{m-1}\} \tag{74}$$

We can estimate further using (69) and the submultiplicativity

$$\|S_m\|^{m-1} = \|e^{-i\frac{t}{m}(A+B)}\|^{m-1} = (e^{\frac{1}{m}|t|\,\|A+B\|_{\mathbb{C}^{n\times n}}})^{m-1} = e^{\frac{m-1}{m}|t|\,\|A+B\|_{\mathbb{C}^{n\times n}}} \leqslant e^{|t|\,\|A+B\|_{\mathbb{C}^{n\times n}}}$$

and (again using (69))

$$\|T_m\|^{m-1} = \|e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B}\|^{m-1} \leqslant \left(\|e^{-i\frac{t}{m}A}\|\,\|e^{-i\frac{t}{m}B}\|\right)^{m-1} = (e^{\frac{1}{m}|t|\,\|A\|_{\mathbb{C}^{n\times n}}}e^{\frac{1}{m}|t|\,\|B\|_{\mathbb{C}^{n\times n}}})^{m-1}$$

$$\leqslant e^{|t|\,(\|A\|_{\mathbb{C}^{n\times n}}+\|B\|_{\mathbb{C}^{n\times n}})}.$$

Using this and (74) we obtain that for some $K > 0$ we have

$$\|S_m^m - T_m^m\| \leqslant \frac{K}{m} \xrightarrow{m\to\infty} 0.$$

Finally we compute that for $m \in \mathbb{N}$, the fact that $\frac{1}{m}(A+B)$ and $\frac{1}{m}(A+B)$ commute implies together with Proposition 4.0.3

$$S_m^m = (e^{-it\frac{1}{m}(A+B)})^m \underset{\text{Prop4.0.3}}{=\!=\!=} e^{-itm\cdot\frac{1}{m}(A+B)} = e^{-it(A+B)}.$$

We obtain

$$\|e^{-it(A+B)} - (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\|_{\mathbb{C}^{n\times n}} \xrightarrow{m\to\infty} 0,$$

as claimed.

4.0.2 The infinite-dimensional case

This theorem *and its proof* can (with some modifications) be generalized to the case of infinite dimensions for self-adjoint operators.

Theorem 4.0.5 — The Trotter-Kato Formula

Let $A : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ and $B : D(B) \to L^2(\mathbb{R}^d;\mathbb{C})$ be two self-adjoint operators and suppose that $A + B : D(A) \cap D(B) \to L^2(\mathbb{R}^d;\mathbb{C})$ is self-adjoint. Then for each $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$ and $t \in \mathbb{R}$ we have

$$e^{-it(A+B)}\varphi = \operatorname*{LIM}_{m\to\infty}\left(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B}\right)^m\varphi. \tag{75}$$

(Recall that $\operatorname*{LIM}_{m\to\infty}$ is to be understood as limit of L^2-functions)

Before we prove this theorem we need a preparatory lemma about the domain of self-adjoint operators, which is of independent interest.

Lemma 4.0.6

Suppose that $A : D(A) \to L^2(\mathbb{R}^d;\mathbb{C})$ is a self-adjoint operator and $D(A)$ be dense[a] in

$L^2(\mathbb{R}^d;\mathbb{C})$. Then

(i) A is *closed* on $D(A)$, i.e. if $(\varphi_n)_{n\in\mathbb{N}} \subseteq D(A)$ is such that $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$ and $A\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} g$ for some $\varphi, g \in L^2(\mathbb{R}^d;\mathbb{C})$ then $\varphi \in D(A)$ and $g = A\varphi$.

(ii) The vector space $D(A)$, endowed with the norm $\|\varphi\|_{D(A)} := \|\varphi\|_{L^2} + \|A\varphi\|_{L^2}$, forms a *Banach space* (i.e. it is *complete* with respect to $\|\cdot\|_{D(A)}$).

[a]Actually, we already require in Definition 3.2.13 that the the domain of any self-adjoint operator has to be dense, so we would not have to include this prerequsite. However, to be consistent with the literature we include it here (since other literature does not require density of the domain for the definition of self-adjointness).

Proof. We start with (i). Let $(\varphi_n)_{n\in\mathbb{N}} \subseteq D(A)$ and $\varphi, g \in L^2(\mathbb{R}^d;\mathbb{C})$ be such that

$$\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi, \qquad A\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} g.$$

We first show that $\varphi \in D(A)$. Using Definition 3.2.13(ii) it suffices to show that there exists $C > 0$ with the property that

$$|\langle A\eta, \varphi\rangle| \leqslant C\|\eta\|_{L^2} \qquad \text{for all } \eta \in D(A).$$

To this end let $\eta \in D(A)$. Then we have (due to symmetry of A, the convergences we have and the Cauchy-Schwarz inequality)

$$|\langle A\eta, \varphi\rangle| = \lim_{n\to\infty} |\langle A\eta, \varphi_n\rangle| = \lim_{n\to\infty} |\langle \eta, A\varphi_n\rangle| = |\langle \eta, g\rangle| \leqslant \|\eta\|_{L^2}\|g\|_{L^2}.$$

The claim follows with $C := \|g\|_{L^2}$ (and as stated above Definition 3.2.13(ii) implies that $\varphi \in D(A)$). It remains to show that $g = A\varphi$. To this end we compute first that for each $\eta \in D(A)$ we have

$$\langle A\varphi, \eta\rangle = \langle \varphi, A\eta\rangle = \lim_{n\to\infty}\langle \varphi_n, A\eta\rangle = \lim_{n\to\infty}\langle A\varphi_n, \eta\rangle = \langle g, \eta\rangle.$$

In particular $\langle A\varphi - g, \eta\rangle = 0$ for all $\eta \in D(A)$. Now, since $D(A)$ is dense in $L^2(\mathbb{R}^d;\mathbb{C})$ take $(\eta_n)_{n\in\mathbb{N}} \subseteq D(A)$ such that $\eta_n \xrightarrow{L^2(\mathbb{R}^d;\mathbb{C})} A\varphi - g$. As a result we have

$$\langle A\varphi - g, A\varphi - g\rangle = \lim_{n\to\infty}\langle A\varphi - g, \eta_n\rangle = \lim_{n\to\infty} 0 = 0,$$

and thus $\|A\varphi - g\|_{L^2} = 0$, i.e. $A\varphi = g$.

Now we turn to (ii). It is clear by definition that $D(A)$ is a vector space. We leave it as an exercise to show that $\|\cdot\|_{D(A)}$ is a norm. Now it remains to show that $(D(A), \|\cdot\|_{D(A)})$ is complete. Let $(\varphi_n)_{n\in\mathbb{N}} \subseteq D(A)$ be a Cauchy sequence with respect to $\|\cdot\|_{D(A)}$. One is readily convinced that then $(\varphi_n)_{n\in\mathbb{N}}$ and $(A\varphi_n)_{n\in\mathbb{N}}$ are Cauchy sequences in $L^2(\mathbb{R}^d;\mathbb{C})$.[a] Since $L^2(\mathbb{R}^d;\mathbb{C})$ is complete we find limits $\varphi, g \in L^2(\mathbb{R}^d;\mathbb{C})$ such that $\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} \varphi$ and $A\varphi_n \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{n\to\infty} g$. By (i) we have $\varphi \in D(A)$ and $A\varphi = g$. This implies

$$\begin{aligned}
\|\varphi_n - \varphi\|_{D(A)} &= \|\varphi_n - \varphi\|_{L^2} + \|A(\varphi_n - \varphi)\|_{L^2} \\
&= \|\varphi_n - \varphi\|_{L^2} + \|A\varphi_n - A\varphi\|_{L^2} \\
&= \|\varphi_n - \varphi\|_{L^2} + \|A\varphi_n - g\|_{L^2} \xrightarrow{n\to\infty} 0 + 0 = 0.
\end{aligned}$$

As a result $(\varphi_n)_{n\in\mathbb{N}}$ is convergent with respect to $\|\cdot\|_{D(A)}$. Completeness of $D(A)$ with respect to $\|\cdot\|_{D(A)}$ is shown.

[a] Indeed, let $\varepsilon > 0$. Due to the fact that $(\varphi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence with respect to $\|\cdot\|_{D(A)}$ we find that

$$\exists n_0 \in \mathbb{N} : \qquad \forall n, m \geqslant n_0 : \qquad \|\varphi_n - \varphi_m\|_{D(A)} < \varepsilon.$$

Now observe that for $m, n \in \mathbb{N}$ we have $\|\varphi_n - \varphi_m\|_{L^2} \leqslant \|\varphi_n - \varphi_m\|_{D(A)}$ and $\|A\varphi_n - A\varphi_m\|_{L^2} = \|A(\varphi_n - \varphi_m)\|_{L^2} \leqslant \|\varphi_n - \varphi_m\|_{D(A)}$. As a result we obtain that (for n_0 chosen as above)

$$\forall n, m \geqslant n_0 : \qquad \|\varphi_n - \varphi_m\|_{L^2} < \varepsilon$$

and

$$\forall n, m \geqslant n_0 : \qquad \|A\varphi_n - A\varphi_m\|_{L^2} < \varepsilon.$$

This shows the claimed Cauchy property.

Before we start the proof we will also recall the *Uniform Boundedness principle*. To this end we recall some notation. For two Banach spaces X and Y we denote by $\mathcal{L}(X,Y)$ the set of all continuous linear operators. For $T \in \mathcal{L}(X,Y)$ we define the *operator norm*

$$\|T\|_{\mathcal{L}(X,Y)} := \sup_{f\in X: f\neq 0} \frac{\|Tf\|_Y}{\|f\|_X},$$

which is a finite number if and only if $T \in \mathcal{L}(X,Y)$. One is readily convinced that $\|\cdot\|_{\mathcal{L}(X,Y)}$ defines a norm on $\mathcal{L}(X,Y)$ and

$$\forall f \in X : \qquad \|Tf\|_Y \leqslant \|T\|_{\mathcal{L}(X,Y)} \|f\|_X.$$

Theorem 4.0.7 — UNIFORM BOUNDEDNESS PRINCIPLE

Let X, Y be Banach spaces and $\mathcal{F} \subseteq \mathcal{L}(X,Y)$ be any set of linear and continuous operators. If

$$\forall x \in X \qquad \sup\{\|Tx\|_Y : T \in \mathcal{F}\} < \infty$$

then

$$\sup\{\|T\|_{\mathcal{L}(X,Y)} : T \in \mathcal{F}\} < \infty$$

We are now ready to prove the Trotter-Kato-Formula.

Proof (of Theorem 4.0.5). Let $A : D(A) \to L^2(\mathbb{R}^d; \mathbb{C})$ and $B : D(B) \to L^2(\mathbb{R}^d; \mathbb{C})$ be as in the statement. Define $D := D(A) \cap D(B)$. Recall that A is the generator of the SCU-group $(e^{-itA})_{t\in\mathbb{R}}$ and B is the generator of the SCU-group $(e^{-itB})_{t\in\mathbb{R}}$. Note that for $\varphi \in D$ and $s \in \mathbb{R}\backslash\{0\}$ we have (due to Definition 3.2.6)

$$\frac{1}{s}(e^{-isA}e^{-isB}\varphi - \varphi) = \frac{1}{s}(e^{-isA}\varphi - \varphi) + \frac{1}{s}e^{-isA}(e^{-isB}\varphi - \varphi) \tag{76}$$

By Definition 3.2.6 the first summand tends to $-iA\varphi$ in $L^2(\mathbb{R}^d; \mathbb{C})$ as $s \to 0$ (since A is the generator of $(e^{-itA})_{t\in\mathbb{R}}$, $(*)$). Hence the L^2-convergence of the first summand in (76) is readily understood. We will now examine the second summand, which is a tiny bit more involved. First note that for the same reason as in $(*)$ we have that $\frac{e^{-isB}\varphi-\varphi}{s} \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{s\to 0} -iB\varphi$ as $s \to 0$. Now we may write

$$\frac{1}{s}e^{-isA}(e^{-isB}\varphi - \varphi) = e^{-isA}\left(\frac{e^{-isB}\varphi - \varphi}{s} + iB\varphi\right) - e^{-isA}iB\varphi. \tag{77}$$

The last summand tends to $-iB\varphi$ in $L^2(\mathbb{R}^d; \mathbb{C})$ as $s \to 0$ by Axiom (U2) of Definition 3.2.1. For the first summand we compute (using the unitariness)

$$\left\| e^{-isA}\left(\frac{e^{-isB}\varphi - \varphi}{s} + iB\varphi\right)\right\|_{L^2} = \left\|\frac{e^{-isB}\varphi - \varphi}{s} + iB\varphi\right\|_{L^2} \xrightarrow{s\to 0} 0.$$

In particular, the whole expression in (77) goes to $-iB\varphi$ and thus (76) yields

$$\frac{1}{s}(e^{-isA}e^{-isB}\varphi - \varphi) \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{s\to 0} -iA\varphi - iB\varphi = -i(A + B)\varphi. \tag{78}$$

Due to the fact that $A + B$ generates the SCU-group $(e^{-it(A+B)})_{t\in\mathbb{R}}$ we also have

$$\frac{1}{s}(e^{-is(A+B)}\varphi - \varphi) = -i(A + B)\varphi \qquad (s \to 0).$$

We can now define for $s \in \mathbb{R}\backslash\{0\}$ the linear operator $K(s) := \frac{1}{s}(e^{-isA}e^{-isB} - e^{-is(A+B)}) : D \to L^2(\mathbb{R}^d; \mathbb{C})$ and infer from the last two equations that[a]

$$\forall\varphi \in D : \qquad K(s)\varphi \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{s\to 0} 0 \tag{79}$$

Intermediate claim 1. If D is endowed with the norm $\|\varphi\|_D := \|\varphi\|_{L^2} + \|(A + B)\varphi\|_{L^2}$ (see Lemma 4.0.6) then $\sup\{\|K(s)\|_{\mathcal{L}(D,L^2)} : s \in \mathbb{R}\backslash\{0\}\} < \infty$

To this end note first that D is a Banach space w.r.t. $\|\cdot\|_D$ by Lemma 4.0.6 (and the prerequisite that $A+B$ is self-adjoint). We seek to apply the uniform boundedness principle to $X = D, Y = L^2(\mathbb{R}^d;\mathbb{C})$ and $\mathcal{F} := \{K(s) : s \in \mathbb{R}\backslash\{0\}\}$. First note that in this case $\mathcal{F}$ contains only linear and continous operators, since for each $s \in \mathbb{R}$ and $\varphi_0 \in D$ we have

$$\begin{aligned}\|K(s)\varphi_0\|_{L^2} &= \frac{1}{|s|}\|(e^{-isA}e^{-isB} - e^{-is(A+B)})\varphi_0\|_{L^2} \\ &\leqslant \frac{1}{|s|}(\|e^{-isA}e^{-isB}\varphi_0\|_{L^2} + \|e^{-is(A+B)}\varphi_0\|_{L^2}) \\ &\underset{\text{(U1) in Def3.2.1}}{=\!=\!=\!=\!=} \frac{1}{|s|}(\|\varphi_0\|_{L^2} + \|\varphi_0\|_{L^2}) = \frac{2}{|s|}\|\varphi_0\|_{L^2} \leqslant \frac{2}{|s|}\|\varphi_0\|_D. \quad (80)\end{aligned}$$

This implies that for each $s \in \mathbb{R}\backslash\{0\}$ the operator $K(s) : D \to L^2(\mathbb{R}^d;\mathbb{C})$ is linear and bounded with operator norm $\|K(s)\|_{\mathcal{L}(D,L^2)} \leqslant \frac{2}{|s|}$. Next we will show that for each $\varphi_0 \in D$ we have $S_{\varphi_0} := \sup\{\|K(s)\varphi_0\|_{L^2} : s \in \mathbb{R}\backslash\{0\}\} < \infty$. To this end fix $\varphi_0 \in D$ and let $(s_n)_{n\in\mathbb{N}} \subset \mathbb{R}\backslash\{0\}$ be such that $\|K(s_n)\varphi_0\|_{L^2} \xrightarrow{n\to\infty} S_{\varphi_0}$. We distinguish two cases.

Case 1. $s_n \not\longrightarrow 0$ as $n \to \infty$.

In this case we can find a subsequence $(s_{\ell_n})_{n\in\mathbb{N}}$ and $\delta > 0$ such that $|s_{\ell_n}| > \delta$ for all $n \in \mathbb{N}$. Therefore we have

$$S_{\varphi_0} = \lim_{n\to\infty}\|K(s_{\ell_n})\varphi_0\|_{L^2} \underset{(80)}{\leqslant} \liminf_{n\to\infty}\frac{2}{|s_{\ell_n}|}\|\varphi_0\|_D \leqslant \frac{2}{\delta}\|\varphi_0\|_D < \infty.$$

Case 2. $s_n \longrightarrow 0$ as $n \to \infty$

Then by (79) we have

$$S_{\varphi_0} = \lim_{n\to\infty}\|K(s_n)\varphi_0\|_{L^2} = \lim_{n\to\infty}\|K(s_n)\varphi_0 - 0\|_{L^2} = \lim_{s\to 0}\|K(s)\varphi_0 - 0\|_{L^2} = 0 < \infty.$$

We have shown that for all $\varphi_0 \in D$ we have $\sup\{\|K(s)\varphi_0\|_{L^2} : s \in \mathbb{R}\backslash\{0\}\} < \infty$. Thereupon the uniform boundedness principle yields the intermediate claim.

Intermediate claim 2. If $K \subseteq D$ is a compact set then $\lim_{s\to 0}\sup_{\varphi\in K}\|K(s)\varphi\|_{L^2} = 0$.

To this end choose for each $s \in \mathbb{R}\backslash\{0\}$ some $\varphi_s \in K$ such that $\|K(s)\varphi_s\|_{L^2} = \sup_{\varphi\in K}\|K(s)\varphi\|_{L^2}$ (using that this supremum is attained since K is compact). Now let $(s_n)_{n\in\mathbb{N}} \subseteq \mathbb{R}\backslash\{0\}$ be a sequence that converges to 0. Assume for a contradiction that $\|K(s_n)\varphi_{s_n}\|_{L^2} \not\longrightarrow 0$. Then there exists $\delta > 0$ and a subsequence $(\ell_n)_{n\in\mathbb{N}} \subseteq \mathbb{N}$ such that $\|K(s_{\ell_n})\varphi_{s_{\ell_n}}\|_{L^2} \geqslant \delta$ for all $n \in \mathbb{N}$. Possibly choosing a further subsequence we can (due so the fact that $(\varphi_{\ell_n})_{n\in\mathbb{N}} \subset K$ and K is compact) also assume that there exists some $\varphi_0 \in K$ such that $\varphi_{\ell_n} \xrightarrow[D]{n\to\infty} \varphi_0$ (by which we mean $\|\varphi_{\ell_n} - \varphi_0\|_D \xrightarrow{n\to\infty} 0$). Using this we can write

$$K(s_{\ell_n})\varphi_{s_{\ell_n}} = K(s_{\ell_n})(\varphi_{s_{\ell_n}} - \varphi_0) + K(s_{\ell_n})\varphi_0.$$

Now due to (79) we have $\|K(s_{\ell_n})\varphi_0\|_{L^2} \xrightarrow{n\to\infty} 0$. Moreover we have (using Intermediate Claim 1)

$$\begin{aligned}\|K(s_{\ell_n})(\varphi_{s_{\ell_n}} - \varphi_0)\|_{L^2} &\leqslant \|K(s_{\ell_n})\|_{\mathcal{L}(D;L^2)} \ \|\varphi_{s_{\ell_n}} - \varphi_0\|_D \\ &\leqslant \left(\sup_{s' \in \mathbb{R}\setminus\{0\}} \|K(s')\|_{\mathcal{L}(D;L^2)}\| \right) \varphi_{s_{\ell_n}} - \varphi_0\|_D \xrightarrow{n\to\infty} 0.\end{aligned}$$

Intermediate claim 3. Let $\varphi_0 \in D$ and $M \in \mathbb{N}$. Then the set $K := \{e^{-is(A+B)}\varphi_0 : s \in [-M, M]\}$ is compact in D.

To this end we take a sequence in K, say $(e^{-is_n(A+B)}\varphi_0)_{n\in\mathbb{N}}$ where $s_n \in [-M, M]$ for all $n \in \mathbb{N}$. Clearly $(s_n)_{n\in\mathbb{N}} \subset [-M, M]$ has a convergent subsequence $(s_{\ell_n})_{n\in\mathbb{N}}$ whose limit we call $s \in [-M, M]$. We claim that now $\|e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0\|_D \xrightarrow{n\to\infty} 0$. To this end recall that

$$\begin{aligned}&\|e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0\|_D \\ &= \|e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0\|_{L^2} + \|(A+B)(e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0)\|_{L^2}.\end{aligned} \tag{81}$$

We first examine the first summand. Due to the Axioms (U1),(U2),(U3) in Definition 3.2.1 we have

$$\begin{aligned}\|e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0\|_{L^2} &\underset{(\mathrm{U3})}{=} \|e^{-is(A+B)}(e^{-i(s_{\ell_n}-s)(A+B)}\varphi_0 - \varphi_0)\|_{L^2} \\ &\underset{(\mathrm{U1})}{=} \|e^{-i(s_{\ell_n}-s)(A+B)}\varphi_0 - \varphi_0\|_{L^2} \underset{(\mathrm{U2})}{\xrightarrow{n\to\infty}} 0.\end{aligned}$$

For the second summand we compute (using the commutation relation Proposition 3.2.8 (ii))

$$\begin{aligned}&\|(A+B)(e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0)\|_{L^2} \\ &= \|(A+B)e^{-is_{\ell_n}(A+B)}\varphi_0 - (A+B)e^{-is(A+B)}\varphi_0\|_{L^2} \\ &= \|e^{-is_{\ell_n}(A+B)}(A+B)\varphi_0 - e^{-is(A+B)}(A+B)\varphi_0\|_{L^2}\end{aligned}$$

We can now argue exactly as in the previous summand with $\varphi_1 := (A+B)\varphi_0$ in place of φ_0 to find that this expression tends to 0 as $n \to \infty$. Using all these insights in (81) we obtain

$$\lim_{n\to\infty} \|e^{-is_{\ell_n}(A+B)}\varphi_0 - e^{-is(A+B)}\varphi_0\|_D = 0,$$

and the claim follows.

Note that Intermediate claim 2 and 3 together imply that for each $\varphi_0 \in D$ we have

$$\lim_{s\to 0} \sup_{r\in[-M,M]} \|K(s)e^{-ir(A+B)}\varphi_0\|_{L^2} = 0 \tag{82}$$

We will use this later. Now we finally turn to (75). We first argue in the special case that $\varphi = \varphi_0 \in D$. For $m \in \mathbb{N}$ we can write

$$\begin{aligned}
&(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi_0 - (e^{-i\frac{t}{m}(A+B)})^m\varphi_0 \\
&= \sum_{k=0}^{m-1} (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^{k+1}(e^{-i\frac{t}{m}(A+B)})^{m-k-1}\varphi_0 - (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^{k}(e^{-i\frac{t}{m}(A+B)})^{m-k}\varphi_0 \\
&= \sum_{k=0}^{m-1} (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^{k}(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B} - e^{-i\frac{t}{m}(A+B)})(e^{-i\frac{t}{m}(A+B)})^{m-k-1}\varphi_0 \\
&= \sum_{k=0}^{m-1} (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^{k}\tfrac{t}{m}K(\tfrac{t}{m})e^{-i\frac{(m-k+1)t}{m}(A+B)}\varphi_0,
\end{aligned}$$

where we have used the SCU-property (U3) from Definition 3.2.1 in the last step[b]. Using the triangle inequality and (U1) we obtain

$$\begin{aligned}
\|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi_0 - (e^{-i\frac{t}{m}(A+B)})^m\varphi_0\|_{L^2} &\leqslant \sum_{k=0}^{m-1} \tfrac{|t|}{m}\|K(\tfrac{t}{m})e^{-i\frac{(m-k+1)t}{m}(A+B)}\varphi\|_{L^2} \\
&= \sum_{k=0}^{m-1} \tfrac{|t|}{m} \sup_{r\in[-|t|,|t|]} \|K(\tfrac{t}{m})e^{-ir(A+B)}\varphi_0\|_{L^2} \\
&= |t| \sup_{r\in[-|t|,|t|]} \|K(\tfrac{t}{m})e^{-ir(A+B)}\varphi_0\|_{L^2}.
\end{aligned}$$

Due to (82) we find that $\lim_{m\to\infty} \sup_{r\in[-|t|,|t|]} \|K(\frac{t}{m})e^{-ir(A+B)}\varphi\|_{L^2} = 0$. We have hence shown that

$$\operatorname*{LIM}_{m\to\infty} (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi_0 - (e^{-i\frac{t}{m}(A+B)})^m\varphi_0 = 0.$$

Using again the SCU-property (U3) from Definition 3.2.1 we obtain that $(e^{-i\frac{t}{m}(A+B)})^m = e^{-it(A+B)}$ (see also the computation in (83)). This implies

$$\operatorname*{LIM}_{m\to\infty} (e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi_0 = e^{-it(A+B)}\varphi_0.$$

So far we have only looked at the special case $\varphi = \varphi_0 \in D$. We however intend to show the claim for all general $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. To this end we will use that D is dense in $L^2(\mathbb{R}^d;\mathbb{C})$. To this end let $\varphi \in L^2(\mathbb{R}^d;\mathbb{C})$. Fix $\varepsilon > 0$ arbitrary and choose $\varphi_0 \in D$ such that $\|\varphi - \varphi_0\| < \frac{1}{2}\varepsilon$. We compute

$$\|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi - e^{-it(A+B)}\varphi\|_{L^2}$$

$$
\begin{aligned}
&\leqslant \|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi_0 - e^{-it(A+B)}\varphi_0\|_{L^2} \\
&\qquad + \|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m(\varphi-\varphi_0)\|_{L^2} + \|e^{-it(A+B)}(\varphi-\varphi_0)\|_{L^2} \\
&\leqslant \|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi_0 - e^{-it(A+B)}\varphi_0\|_{L^2} + 2\|\varphi-\varphi_0\|_{L^2},
\end{aligned}
$$

where we have used in the last step that all the operators $e^{-i\frac{t}{m}A}, e^{-i\frac{t}{m}B}, e^{-it(A+B)}$ have operator norm equal one due to (U1) (and also that the operator norm is submultiplicative). As a result we obtain (given that the claim is already shown for $\varphi_0 \in D$

$$\limsup_{m\to\infty}\|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi - e^{-it(A+B)}\varphi\|_{L^2} \leqslant 2\|\varphi-\varphi_0\|_{L^2} < 2\cdot\tfrac{1}{2}\varepsilon = \varepsilon.$$

Since $\varepsilon > 0$ was arbitrary we find

$$\limsup_{m\to\infty}\|(e^{-i\frac{t}{m}A}e^{-i\frac{t}{m}B})^m\varphi - e^{-it(A+B)}\varphi\|_{L^2} = 0.$$

The claim follows.

[a]Here we would have to compute for $\varphi \in D$

$$
\begin{aligned}
K(s)\varphi &= \frac{1}{s}(e^{-isA}e^{-isB} - e^{-is(A+B)})\varphi \\
&= \frac{e^{-isA}e^{-isB}\varphi - \varphi}{s} - \left(\frac{e^{-is(A+B)}\varphi - \varphi}{s}\right) \xrightarrow[L^2(\mathbb{R}^d;\mathbb{C})]{s\to 0} -i(A+B)\varphi + i(A+B)\varphi = 0,
\end{aligned}
$$

where we used (78) to pass to the limit in the first summand and the generator property in Definition 3.2.6 in the second summand.

[b]Indeed, for $\ell \in \mathbb{N}$ we have

$$(e^{-i\frac{t}{m}(A+B)})^\ell = \underbrace{e^{-i\frac{t}{m}(A+B)} \circ \ldots \circ e^{-i\frac{t}{m}(A+B)}}_{\ell \text{ times}} \underset{\text{(U3)}}{=} e^{-i(\frac{t}{m}+\ldots+\frac{t}{m})(A+B)} = e^{-i\frac{\ell t}{m}(A+B)}. \tag{83}$$

It should be stressed at this point that this claum does not use any nontrivial commutator law but just (U3).

4.0.3 Application to the Schrödinger equation

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We have seen that the formula in (66) is generally wrong. Still, the Trotter-Kato Formula in Theorem 4.0.5 allows us to express $e^{-iHt} = e^{-i(-\frac{1}{2}\Delta+M_V)t}$ in terms of the known SCU-grops $(e^{-i(-\frac{1}{2}\Delta)t})_{t\in\mathbb{R}}$ and $(e^{-iM_Vt})_{t\in\mathbb{R}}$ (provided that V is as in Proposition 3.2.26 to ensure that H is self-adjoint). Namely, for every $\varphi \in L^2(\mathbb{R}^3;\mathbb{C})$ and $t \in \mathbb{R}$ we have now

$$e^{-itH}\varphi = e^{-it(-\frac{1}{2}\Delta+M_V)}\varphi = \operatorname*{LIM}_{m\to\infty}(e^{-i\frac{t}{m}(-\frac{1}{2}\Delta)}e^{-i\frac{t}{m}M_V})^m\varphi.$$

Using the explicit formulae (64) and (65) we could now approximate $e^{-iHt}\varphi$ as closely as we want. But recall that we want more than that. Indeed, we would like to have a *propagator* satisfying similar properties to the free propagator (like a formula as in Theorem 3.1.13 that allows calculation of ψ_t in terms of the initial value ψ_0). Note that for any $m \in \mathbb{N}$ and

$\varphi_0 \in L^2(\mathbb{R}^3;\mathbb{C})$ and $t \in \mathbb{R}\backslash\{0\}$ we have (for a.e. $x \in \mathbb{R}^d$, writing $\int$ instead of $\tilde{\int}$)

$$[e^{-i\frac{t}{m}(-\frac{1}{2}\Delta)}e^{-i\frac{t}{m}M_V}\varphi_0](x) = [e^{-i\frac{t}{m}(-\frac{1}{2}\Delta)}e^{-i\frac{t}{m}V(\cdot)}\varphi_0(\cdot)](x) = \frac{1}{(2\pi i\frac{t}{m})^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{i\frac{|x-y|^2}{2\frac{t}{m}}}\, e^{-i\frac{t}{m}V(y)}\varphi_0(y)\,\mathrm{d}y$$

$$= \frac{m^{\frac{3}{2}}}{(2\pi it)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{im\frac{|x-y|^2}{2t}}\, e^{-i\frac{t}{m}V(y)}\varphi_0(y)\,\mathrm{d}y.$$

We define thus now $\varphi_1 := e^{-i\frac{t}{m}(-\frac{1}{2}\Delta)}e^{-i\frac{t}{m}M_V}\varphi_0 \in L^2(\mathbb{R}^3;\mathbb{C})$ to be

$$\varphi_1(x) = \frac{m^{\frac{3}{2}}}{(2\pi it)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{im\frac{|x-y|^2}{2t}}\, e^{-i\frac{t}{m}V(y)}\varphi_0(y)\,\mathrm{d}y \qquad \text{for a.e. } x \in \mathbb{R}^3. \tag{84}$$

Notice that $\varphi_m := (e^{-i(-\frac{1}{2}\Delta)\frac{t}{m}}e^{-iM_V\frac{t}{m}})^m\varphi_0$ can now be calculated applying the above operation m times. We will now write this more precisely. Define φ_1 as above and then for $j = 2, ..., m$ form $\varphi_j := e^{-i(-\frac{1}{2}\Delta)\frac{t}{m}}e^{-iM_V\frac{t}{m}}\varphi_{j-1} \in L^2(\mathbb{R}^3;\mathbb{C})$, i.e. by (84)

$$\varphi_j(x) = \frac{m^{\frac{3}{2}}}{(2\pi it)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{im\frac{|x-y|^2}{2t}}\, e^{-i\frac{t}{m}V(y)}\varphi_{j-1}(y)\,\mathrm{d}y \qquad \text{for a.e. } x \in \mathbb{R}^3.$$

We rename the integration variable to be y_{m-j+1} and thus have for a.e. $x \in \mathbb{R}^3$

$$\varphi_j(x) = \frac{m^{\frac{3}{2}}}{(2\pi it)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{im\frac{|x-y_{m-j+1}|^2}{2t}}\, e^{-i\frac{t}{m}V(y_{m-j+1})}\varphi_{i-1}(y_{m-j+1})\,\mathrm{d}y_{m-j+1}$$

Now we calculate explicitly

$$\varphi_1(x) = \frac{m^{\frac{3}{2}}}{(2\pi it)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{im\frac{|x-y_m|^2}{2t}}\, e^{-i\frac{t}{m}V(y_m)}\varphi_0(y_m)\,\mathrm{d}y_m$$

and

$$\begin{aligned}
\varphi_2(x) &= \frac{m^{\frac{3}{2}}}{(2\pi it)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{im\frac{|x-y_{m-1}|^2}{2t}}\, e^{-i\frac{t}{m}V(y_{m-1})}\varphi_1(y_{m-1})\,\mathrm{d}y_{m-1} \\
&= \frac{m^3}{(2\pi it)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} e^{im\frac{|x-y_{m-1}|^2}{2t}}\, e^{-i\frac{t}{m}V(y_{m-1})}e^{im\frac{|y_{m-1}-y_m|^2}{2t}}\, e^{-i\frac{t}{m}V(y_m)}\varphi_0(y_m)\,\mathrm{d}y_m\,\mathrm{d}y_{m-1} \\
&= \frac{m^3}{(2\pi it)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} e^{im\frac{|x-y_{m-1}|^2+|y_{m-1}-y_m|^2}{2t}}\, e^{-i\frac{t}{m}(V(y_{m-1})+V(y_m))}\varphi_0(y_m)\,\mathrm{d}y_m\,\mathrm{d}y_{m-1} \\
&= \frac{m^3}{(2\pi it)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} e^{i\frac{t}{m}\left(\frac{|x-y_{m-1}|^2+|y_{m-1}-y_m|^2}{2(t/m)^2}-V(y_{m-1})-V(y_m)\right)}\varphi_0(y_m)\,\mathrm{d}y_m\,\mathrm{d}y_{m-1}
\end{aligned}$$

Inductively we obtain for a.e. $y_0 \in \mathbb{R}^3$

$$\varphi_m(y_0) = \frac{m^{\frac{3m}{2}}}{(2\pi it)^{\frac{3m}{2}}}\int_{\mathbb{R}^3}\cdots\int_{\mathbb{R}^3} \exp\left(i\frac{t}{m}\sum_{i=1}^{m}\left(\frac{|y_i-y_{i-1}|^2}{2(t/m)^2} - V(y_i)\right)\right)\varphi_0(y_m)\,\mathrm{d}y_m \,...\, \mathrm{d}y_1.$$

Hence we have shown

Proposition 4.0.8

Let $V \in L^2(\mathbb{R}^3;\mathbb{C}) + L^\infty(\mathbb{R}^3;\mathbb{C})$. Then for $H = -\frac{1}{2}\Delta + M_V : W^{2,2}(\mathbb{R}^3;\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C})$ and $\varphi \in L^2(\mathbb{R}^3;\mathbb{C}), t \in \mathbb{R}\backslash\{0\}$ we have

$$e^{-itH}\varphi = \operatorname*{LIM}_{m\to\infty} \frac{m^{\frac{3m}{2}}}{(2\pi i t)^{\frac{3m}{2}}} \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3} \exp\left(iS_m(\cdot, y_1, ..., y_m, t)\right) \varphi(y_m)\, \mathrm{d}y_m \, ... \, \mathrm{d}y_1. \tag{85}$$

where $S_m : \mathbb{R}^{3(m+1)} \times \mathbb{R}\backslash\{0\} \to \mathbb{R}$ is given by

$$S_m(y_0, y_1, ..., y_m, t) := \frac{t}{m} \sum_{j=1}^m \left(\frac{|y_j - y_{j-1}|^2}{2(t/m)^2} - V(y_j) \right). \tag{86}$$

This formula was stated first in 1948 by Feynman on the basis of a physical interpretation. If a classical particle of mass 1 moves along a trajectory $\omega = \omega(s), 0 \leqslant s \leqslant t$ inside a potential V (suitably smooth) it is said to have *action* equal to

$$S(\omega) := \int_0^t \left(\tfrac{1}{2}|\dot{\omega}(s)|^2 - V(\omega(s))\right) \mathrm{d}s$$

Now suppose that $\omega = \omega_{y_0,...,y_m}$ is the piecewise linear interpolation of $y_0, ..., y_m$, that is

- ω is affine linear on $[\frac{(k-1)t}{m}, \frac{kt}{m}]$ for all $k = 1, ..., m$
- $\omega(\frac{kt}{m}) = y_k$

In particular $\dot{\omega}$ is constant on $(\frac{(k-1)t}{m}, \frac{kt}{m})$ and for $s \in (\frac{(k-1)t}{m}, \frac{kt}{m})$ we have

$$\dot{\omega}(s) = \frac{\omega(\frac{kt}{m}) - \omega(\frac{(k-1)t}{m})}{\frac{t}{m}} = \frac{y_k - y_{k-1}}{\frac{t}{m}}$$

This shows that

$$\int_0^t \frac{1}{2}|\dot{\omega}(s)|^2 \,\mathrm{d}s = \sum_{j=1}^m \int_{\frac{(j-1)t}{m}}^{\frac{jt}{m}} \frac{1}{2}|\dot{\omega}(s)|^2 \,\mathrm{d}s = \sum_{j=1}^m \int_{\frac{(j-1)t}{m}}^{\frac{jt}{m}} \frac{1}{2}\frac{|y_j - y_{j-1}|^2}{(t/m)^2} \,\mathrm{d}s = \frac{t}{m}\sum_{j=1}^m \frac{|y_j - y_{j-1}|^2}{2(t/m)^2}.$$

If the potential is not varying too much one could also approximate

$$\int_0^t V(\omega(s)) \,\mathrm{d}s = \sum_{j=1}^m \int_{\frac{(j-1)t}{m}}^{\frac{jt}{m}} V(\omega(s)) \,\mathrm{d}s \approx \sum_{j=1}^m \int_{\frac{(j-1)t}{m}}^{\frac{jt}{m}} V(\omega(\tfrac{jt}{m})) \,\mathrm{d}s = \frac{t}{m}\sum_{j=1}^m V(y_j).$$

As a consequence we obtain

$$S(\omega_{y_0,...,y_m}) \qquad \text{coincides almost with } S_m(y_0, ..., y_m, t) \text{ given as in (86).}$$

Replacing this, the right hand side of (85) reads

$$(e^{-iHt}\varphi)(y_0) = \operatorname*{LIM}_{m\to\infty} \frac{m^{\frac{3m}{2}}}{(2\pi i t)^{\frac{3m}{2}}} \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3} e^{iS(\omega_{y_0,...,y_m})} \varphi(\omega_{y_0,...,y_m}(t))\, \mathrm{d}y_m ... \,\mathrm{d}y_1 \qquad \text{for a.e } y_0 \in \mathbb{R}^3 \tag{87}$$

Having now rewritten the integrand as a function of piecewise continuous paths $\omega_{y_0,\dots,y_m}$ we would like to understand the limit procedure as $m \to \infty$ more closely. It is now reasonable to expect that the limit

$$(e^{-itH}\varphi)(y_0) = \int_\Omega e^{iS(\omega)}\varphi(\omega(t))\, \mathrm{d}\mu_{y_0}(\omega),$$

where Ω is the set of continuous paths on $[0,t]$ and μ_{x_0} is a measure on Ω, the so called *Wiener measure*. This is what physicists call a *path integral*. In reality it should be imagined as nothing but the limit in (87).

This is now the end of the lecture. We hope that we could shed some light on the important mathematical tools and basic concepts of quantum mechanics. We have covered a quite substantial introduction to the time-dependent Schrödinger equation but we have completely ignored the time-independent Schrödinger equation. A more thorough lecture would probably also address this topic and also give a proof of Stone's Theorem (Theorem 3.2.12). In order to do so, one needs *spectral theory of self-adjoint operators*, which would certainly be a natural extension of the present course. For now, we thank the readers very much for their interest and patience!