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V O R L E S U N G

zum Thema

Mathematische Grundlagen der Quantenmechanik

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Inhaltsverzeichnis

1 Introduction: Why this lecture?

Physics and mathematics are related fields, In particular, this holds true for quantum mechanics and functional analysis, which both were founded at the beginning of the 20$^{\text{th}}$ century and are developed since then.

Historically, quantum mechanics started with the discovery of Planck's law of radiation (1900) and Einstein's explanation of the photoeffect (1905). Until around 1920 the so-called "old quantum mechanics" was developed by Bohr, Sommerfeld, Born and others, who explained in particular the atomic spectra (Bohr atomic model). The formalisation of quantum mechanics started in the mid-1920s, particularly by Erwin Schrödinger's wave mechanics and Werner Heisenberg's matrix mechanics, later by Paul Dirac in the 1930s. The mathematical foundations were laid by John von Neumann in 1932.[1] Later in the 1940s quantum field theory was developed, which we shall not consider in this lecture. Quantum mechanics and its foundations have been questioned over and over again, and starting from the 1980s quantum information theory gives rise to new interest in quantum-mechanical foundations.

We shall start this lecture by two examples which show that quantum mechanics differs from classical physics: the first experiment has historically proven that certain quantities are quantised, the second is a *Gedankenexperiment* showing the incompatibility of certain classical reasoning with quantum mechanics.

1.1 The Stern-Gerlach experiment

[...]

1.2 Bell's inequality

[...]

2 The formalism of quantum mechanics

We shall introduce quantum mechanics in this lecture by five postulates and will then present some elementary aspects of quantum mechanics.

[1] Note that the title of this lecture is the title of John von Neumann's book from 1932.

2.1 Postulates of quantum mechanics

There is a variety of approaches to quantum mechanics such as wave mechanics, path integrals, phase spaces etc., but none of this is a priory the right one. Here, we use a well-known approach by introducing five postulates of quantum mechanics; we should note here that there are different versions of these postulates used by different authors, in particular, they should not be understood as mathematical axioms, but rather as guidelines.

Postulate 1 (Hilbertraum)**.**
To every physical system there is associated a complex Hilbert space $\mathcal{H}$.

Now and for the rest of this lecture, $\mathcal{H}$ shall always denote a complex Hilbert space. At this point it is not clear how to associate a Hilbert space to a physical system, which will be discussed later.

Already at this point we should make some comments on notation, which often differs in mathematics and physics. First, abstract vectors in a Hilbert space (elements of $\mathcal{H}$) are written in the form $|\Psi\rangle$ and called *ket vectors*. Vectors in the dual space $\mathcal{H}'$ of $\mathcal{H}$ are functionals on $\mathcal{H}$ and are written as $\langle\varphi|$ and called *bra vectors*; the bra vector acts upon a ket vactor to yield $\langle\varphi|\psi\rangle \in \mathbb{C}$. This notation is called Dirac or bra-ket notation, where *bra-c-ket* is the inner product; a vector and its dual are so a „half“ inner product). The mathematical justification for this notation is the Riesz-Fréchet theorem. In the same fashion $|\varphi\rangle\langle\psi|$ is understood as the mappting $|x\rangle \mapsto \langle\psi|x\rangle \cdot |\varphi\rangle$; in particular, if $|\psi\rangle$ is normalised, then $|\psi\rangle\langle\psi|$ is a projector on the one-dimensional subspace generated by $|\psi\rangle$. Note further, the following differences in notation:

- In physics, the inner product is linear in the second argument, in mathematics usually in the first (and skew-linear in the other).
- The complex conjugate of $z \in \mathbb{C}$ is denoted z^* in physics and $\overline{z}$ in mathematics; the adjoint of an operator A is denoted by $A^\dagger$ in physics and A^* in mathematics.

We can distinguish two types of Hilbert spaces: finite-dimensional and infinite-dimensional. The finite-dimensional complex Hilbert spaces are essentially given by $\mathbb{C}^d$ with the canonical inner product and their elements can be represented by column vectors. Functionals on these spaces are row vectors, operators are matrices, and we can use the methods from linear algebra. Infinite-dimensional Hilbert spaces such as $L^2(\mathbb{R}^n)$ are the realm of functional analysis; there are similarities to linear algebra, but also subtle differences.

The next two postulates deal with the description of measureable quantities and states of a system.

Postulate 2 (Observables)**.**
Measureable quantities (physical variables or observables) are described by selfadjoint operators on $\mathcal{H}$; possible values (measurement outcomes) of an observable $\hat{A}$ are its eigenvalues or, more generally, its spectrum.

In physics, operators are commonly denoted by a hat, e. g. $\hat{A}$, but we will not use this notation consistently. It is not said that every selfadjoint operator corresponds to a measureable quantity, though, we will sometimes assume this. The principal reason for using operators is that operators need not commute. Depending on whether two observables $\hat{A}$ and $\hat{B}$ commute, the quantities they represent are jointly measureable or not (note that matrices commute, if they can be put into diagonal form simultaneously).

Postulate 3 (States)**.**
The state of a physical system is described by a density operator (or statistical operator) ρ on $\mathcal{H}$. This operator is positive semidefinite and trace-normalised (i. e. $\operatorname{Tr}\rho = 1$). The expectation value of a measurement of an observable $\hat{A}$ given this state is $\langle A\rangle = \operatorname{Tr}\rho\hat{A}$.

The density operator may be understood as a generalisation of a probability distribution; in particular, the expectation value of the identity operator is 1. By the trace formula it yields the expectation values of all possible observables. Thus, quantum mechanics is a theory of measureable quantities.

In finite-dimensional systems ($\dim\mathcal{H} = d$) the density operator becomes a density matrix which can be diagonalised and decomposed, not necessarily uniquely, into projection operators:

$$\rho = \sum\nolimits_{k=1}^{d} \lambda_i |\Psi_k\rangle\langle\Psi_k|, \tag{1}$$

where $\lambda_k \geq 0$ and $\sum_{k=1}^{k} \lambda_k = 1$. A special case is $\rho = |\Psi\rangle\langle\Psi|$, i. e. ρ is a one-dimensional projection; in this case the state is called *pure*, otherwise *mixed*. The *state vector* $|\Psi\rangle$ is unique up to a global phase $\mathrm{e}^{\mathrm{i}\varphi}$. It is often easier to work with the state vector than with the density operator (and we will do so), but the properties of the density operator follow from the decomposition above. We mention some more terminology:

- In physics (unlike in mathematics) one does not strictly distinguish between states and state vectors for pure states.
- Given two (or more) state vectors $|\psi\rangle$ and $|\varphi\rangle$, in physics one talks of coherent and incoherent superpositions: coherent superpositions are superpositions of vectors $|\psi\rangle + |\varphi\rangle$, incoherent those of density operators $|\psi\rangle\langle\psi| + |\varphi\rangle\langle\varphi|$ (appropriately renormalised).

- The spectrum is invariant under unitary transformations, and one can consider observables and states in different bases without changing measureable quantities: for a unitary operator U there holds $\operatorname{Tr}\rho\hat{A} = \operatorname{Tr}(U\rho U^\dagger \cdot U\hat{A}U^\dagger)$.

- The state vector is also called „wave function“.

Having described observables and states, we should consider *dynamics* (time evolution) of states and operators. Since the essential quantities of quantum mechanics are expectation values, we can distinguish two so-called pictures of quantum mechanics: the *Schrödinger picture*, where the states change in time, but the operators do not, and the *Heisenberg picture*, where it is the opposite. The Schrödinger picture is the more common one.

There are essentially two ways of how a state can change in time: a continuous evolution by the Schrödinger equation and an instantaneous change by measurements.

Postulate 4 (Time evolution)**.**
The time evolution of a state vector $|\Psi\rangle$ is described by the Schrödinger equation $\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$, where $\hat{H}$ is the selfadjoint the Hamiltonian operator.

The Hamiltonian operator is the operator analog of the energy; in particular, $\langle\hat{H}\rangle$ is the expectation value of the energy of the system. If there are external forces, $\hat{H}$ may depend on time, but we shall not consider this here. The formal solution of the Schrödinger equation is $|\Psi\rangle_t = U(t)|\Psi\rangle_0$ with the unitary operator $U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}$, which itself fulfils the Schrödinger equation; note that $U(t=0) = \mathbb{1}$ and $U(t_1)U(t_2) = U(t_1+t_2)$ hold.

For a density operator, the time evolution formally reads $\rho_t = U(t)\rho_0 U(t)^\dagger$, and the Schrödinger equation is replaced by the von-Neumann equation $\mathrm{i}\hbar\frac{\partial\rho}{\partial t} = [\hat{H},\rho]$. If we want to use the Heisenberg picture instead of the Schrödinger picture, we have to transform the operators instead of the states, but the expectation values of the observables should stay the same: $\langle A\rangle = \operatorname{Tr} U\rho U^\dagger \cdot \hat{A} = \operatorname{Tr}\rho\cdot U^\dagger\hat{A}U$. Therefore the Heisenberg operators are $\hat{A}_H(t) = U(t)^\dagger\hat{A}U(t)$, which fulfil the Heisenberg equations of motions $\mathrm{i}\hbar\frac{\partial\hat{A}_H}{\partial t} = [\hat{A}_H,\hat{H}]$.

While the time evolution by a Hamiltonian operator is in principle reversible, this is not the case for state changes due to measurements (known as „collapse of the wave function“). For simplicity we shall formulate the measurement postulate in terms of finite-dimensional systems only; the general case is similar, but needs more functional analysis.

Postulate 5 (Measurements)**.**
If on a state ρ an observable $\hat{A} = \sum_i \lambda_i P_i$ is measured, where the P_i are

projections on orthogonal eigenspaces with distinct eigenvalues λ_i, a specific outcome λ_k is measured with probability $\operatorname{Tr}\rho P_k$*, and in this case the state is instantaneously transformed into* $\rho_k = \frac{P_k \rho P_k}{\operatorname{Tr}\rho P_k}$.

We have here the intrinsic statistics of quantum mechanics: given two observables with no common eigenspace, the state ρ cannot jointly give deterministic values to both observables. For measurement statistics (but not for dynamics) it is the decomposition of the operator into eigenspaces, rather than the spectrum itself, which is relevant.

Note that measurements can be repeated. If measuring the same observable once again (and no other measurement has occured inbetween) the outcome is the same, and the state does not change. A measurement is therefore also a preparation of a state.

2.2 Modelling a quantum system

We have not yet considered which Hilbert space to use for a given quantum system. Although there is no precise theorem for that, we can formulate the following rule: $\dim \mathcal{H}$ cannot be less than the number of possible outcomes.

We have seen that the Stern-Gerlach experiment produces two measurement outcomes: "up" and "down" for each possible measurement direction; so we choose the Hilbert space of the spin-1/2 particle to be $\mathbb{C}^2$, and we model the measurement in the z-direction by $\sigma_z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ with eigenvalues ± 1 (we ignore prefactors of $\hbar/2$ here) and eigenvectors

$$|z,+\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |z,-\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2}$$

Now, as the x-direction should have exactly the same properties, we need another matrix with the same eigenvalues, but other eigenvectors $|x,+\rangle$ and $|x,-\rangle$, such that $|\langle x,\pm|z,\pm\rangle|^2 = 1/2$. All such matrices can be obtained by rotating σ_z by some U, which (up to irrelevant global phases) is given by

$$U = \begin{pmatrix} \cos\frac{\vartheta}{2} & -\sin\frac{\vartheta}{2}\mathrm{e}^{-\mathrm{i}\varphi} \\ \sin\frac{\vartheta}{2}\mathrm{e}^{\mathrm{i}\varphi} & \cos\frac{\vartheta}{2} \end{pmatrix} \Rightarrow U\sigma_z U^\dagger = \begin{pmatrix} \cos\vartheta & \mathrm{e}^{-\mathrm{i}\varphi}\sin\vartheta \\ \mathrm{e}^{\mathrm{i}\varphi}\sin\vartheta & -\cos\vartheta \end{pmatrix} \tag{3}$$

We can write $\vec{r} = (x,\, y,\, z) \in \mathbb{R}^3$ in polar coordinates by $r \in \mathbb{R}_0^+$, $\vartheta \in [0;\, \pi]\times$ and $\varphi \in [0;\, 2\pi]$ as

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = r \begin{pmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{pmatrix}. \tag{4}$$

Assuming $r = 1$, we see that every space direction gives a matrix $U\sigma_z U^\dagger$ with eigenvalues ± 1; in particular, we find the Pauli matrices $\sigma_x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $\sigma_y = \left(\begin{smallmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{smallmatrix}\right)$, $\sigma_z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ and find that they consistently describe the measurements in the Stern-Gerlach experiment.

2.3 More general systems: position and momentum

In the same fashion as the Stern-Gerlach experiment, we can, in principle, describe any two-level (or spin-1/2) system. Similarly, we can describe systems with $d \in \mathbb{N}$ possible measurement outcomes by using the Hilbert space $\mathcal{H} = \mathbb{C}^d$. Nevertheless, the spin and has no classical analogon and the assumption of finitely many results may seem artificial. We shall thus consider more natural systems.

2.3.1 Classical mechanics

In classical mechanics, a state of a system is described by a point in phase space, which takes the place of the Hilbert space in quantum mechanics. For a point-like particle the phase space is $\mathbb{R}^3 \times \mathbb{R}^3$, where the components $(\vec{r}, \vec{p}) = (x, y, z, p_x, p_x, p_x)$ describe position and momentum in a cartesian coordinate system. The time evolution of the state is described e. g. by the Hamiltonian equations of motions, which are first-order in time and define trajectories in phase space (see later). The analogon of a mixed state would be a probability density (instead of a point-like probability) in phase space.

We want to model this system quantum-mechanically. We shall often restrict our consideration to a particle movement in one direction, so that we are left with just one position x and one momentum p. Since the possible outcomes of both position and momentum lie on the real line and are continuous, we need an infinite-dimensional Hilbert space.

2.3.2 Canonical quantisation

Classically, every quantity of a physical system can be expressed in terms of position and momentum, and a rule termed *canonical quantisation* states that commutator of the operators of these quantities should fulfil $[\hat{x}, \hat{p}] := \hat{x}\hat{p} - \hat{p}\hat{x} = \mathrm{i}\hbar \mathbb{1}_{\mathcal{H}}$ (in more that one dimension this would read $[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}\mathbb{1}$).

Exercise 6 (Commutators and traces)**.**
What is wrong with the following reasoning?

1. *For A and B, there holds* $\operatorname{Tr} AB = \operatorname{Tr} BA$ *by the coordinate representation of matrices. This can be rewritten as* $\operatorname{Tr}[A, B] = 0$.

2. *For* $[\hat{x}, \hat{p}] = \mathrm{i}\hbar\mathbb{1}_{\mathcal{H}}$*, this implies* $0 = \mathrm{i}\hbar \dim \mathcal{H}$ *or* $\dim \mathcal{H} = 0$*, i. e. there is no quantum mechanics.*

But we can try the following: on $\mathcal{H} = L^2(\mathbb{R})$, or strictly speaking on an appropriate dense subset thereof, let $\hat{x}$ be the multiplication operator, i. e. $(\hat{x}f)(x) := x \cdot f(x)$, and let $\hat{p} := \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$. For any appropriate function f, there holds

$$\left(x\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x} - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}x\right) f(x) = \frac{\hbar}{\mathrm{i}}\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right) f(x) = \frac{\hbar}{\mathrm{i}}\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x - x\frac{\partial}{\partial x}f(x)\right) = \mathrm{i}\hbar f,$$

i. e. the canonical commutation relation $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$. Since $\hat{x}$ is a multiplication operator, this is called the *position representation*. We could also choose (for functions $g(p)$) $\hat{p}$ to be a multiplication operator, $\hat{p} = p\cdot$, and $\hat{x} := \mathrm{i}\hbar\frac{\partial}{\partial p}$, the *momentum representation*. Essentially, this is a change of bases by a Fourier transform.

2.3.3 Eigenvalues and eigenvectors

In the finite-dimensional case, a number $\lambda \in \mathbb{C}$ is an eigenvalue of a matrix A, if and only if $\lambda\mathbb{1} - A$ is singular. So we may ask about the eigenvalues of $\hat{x}$ and $\hat{p}$.

For $\psi_k(x) := \mathrm{e}^{\mathrm{i}kx}$ for $k \in \mathbb{R}$ and the momentum operator, we calculate $\hat{p}\psi(x) = \hbar k\psi(x)$, so every real number is an eigenvalue of $\hat{p}$ and in the spectrum of $\hat{p}$. But this reasoning is not correct, since none of the ψ_k is square-integrable. For the position operator $\hat{x}$ we can also find formal solutions to the eigenvector problem $(\hat{x}\psi)(x) = a\psi(x)$ for every $a \in \mathbb{R}$, namely "delta functions" δ_a, defined by the property that $\delta_a(x) = 0$ for $x \neq a$ and $\int_{x\in\mathbb{R}} \delta_a(x)\,\mathrm{d}x = 1$. Measure theory tells us that no such function exists, but if it did exist, it would be a solution.

Consider, however, L^2-normalised functions $\varphi_n(x) := (2n/\pi)^{1/4}\mathrm{e}^{-nx^2}$. Then $\lim_{n\to\infty}(\lambda\mathbb{1}-\hat{x})\varphi_n(x-\lambda) = 0$—as it would be, if $\varphi_n(x-\lambda$ were eigenfunctions. If we could exchange limit and operator, we would find $\lim_{n\to\infty}\varphi_n^2(x-\lambda) = \delta_\lambda(x)$. With this in mind, we call λ an *approximative eigenvalue* of $\hat{x}$.

Functional analysis will tell us that the spectra of $\hat{x}$ and $\hat{p}$ are indeed $\mathbb{R}$, and that for self-adjoint operators, the spectrum consists of eigenvalues and approximative eigenvalues only. The notion of a delta function will be made precise in the theory of distributions.

2.4 Uncertainty relations

Given an observable $\hat{A}$, we can—in the sense of classical statistics—speak of it moments, in particular, its *expectation value* $\mathcal{E}(\hat{A}) = \langle\hat{A}\rangle$ and its *variance*

$\mathrm{Var}(\hat{A}) = (\Delta\hat{A})^2 = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$; the *standard deviation* is the square root of the variance $\Delta\hat{A} = \sqrt{(\Delta\hat{A})^2}$. Let us for the sake of simplicity assume that $\langle\hat{A}\rangle = \langle\hat{B}\rangle = 0$ (otherwise one could shift the observable accordingly) and consider an arbitrary pure state $|\Psi\rangle$. We calculate

$$
\begin{aligned}
(\Delta\hat{A})^2(\Delta\hat{B})^2 &\geq \left|\langle\hat{A}\Psi|\hat{B}\Psi\rangle\right|^2 = \left|\mathrm{Re}\,\langle\hat{A}\Psi|\hat{B}\Psi\rangle + \mathrm{i}\,\mathrm{Im}\,\langle\hat{A}\Psi|\hat{B}\Psi\rangle\right|^2 && (5)\\
&= \left|\mathrm{Re}\,\langle\hat{A}\Psi|\hat{B}\Psi\rangle\right|^2 + \left|\mathrm{Im}\,\langle\hat{A}\Psi|\hat{B}\Psi\rangle\right|^2 && (6)\\
&= \left|\frac{\langle\hat{A}\Psi|\hat{B}\Psi\rangle + \langle\hat{B}\Psi|\hat{A}\Psi\rangle}{2}\right|^2 + \left|\frac{\langle\hat{A}\Psi|\hat{B}\Psi\rangle - \langle\hat{B}\Psi|\hat{A}\Psi\rangle}{2\mathrm{i}}\right|^2 && (7)\\
&= \frac{1}{4}\left(\left|\langle\Psi|\{\hat{A},\,\hat{B}\}|\Psi\rangle\right|^2 + \left|\langle\Psi|[\hat{A},\,\hat{B}]|\Psi\rangle\right|^2\right) && (8)\\
&= \frac{1}{4}\left(\left|\langle\{\hat{A},\,\hat{B}\}\rangle\right|^2 + \left|\langle[\hat{A},\,\hat{B}]\rangle\right|^2\right), && (9)
\end{aligned}
$$

where $[\hat{A},\,\hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator and $\{\hat{A},\,\hat{B}\} := \hat{A}\hat{B} + \hat{B}\hat{A}$ the anticommutator of $\hat{A}$ and $\hat{B}$. This is known as Schrödinger's uncertainty relation.

Since both terms are non-negative, we can ignore the first term and take the square root to get the Robertson relation $\Delta\hat{A}\Delta\hat{B} = \frac{1}{2}\left|\langle[\hat{A},\,\hat{B}]\rangle\right|$. Futher, for $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$ with $[\hat{x},\,\hat{p}] = \mathrm{i}\hbar$, we get the Kennard-Heisenberg relation $\Delta\hat{A}\Delta\hat{B} \geq \frac{\hbar}{2}$.

2.5 Mathematical aspects

We have constructed operators $\hat{x}$ and $\hat{p}$, which fulfil the canonical commutation relation. Now we have to ask whether the construction is unique in the sense that their spectrum is already determined by the canonical commutation relations. This is not the case.

Consider the Hilbert space $L^2_{\mathrm{per}}[-a;\,a]$ restricted to periodic functions, i. e. $\psi(-a) = \psi(a)$, with formally the same operators $\hat{x}$ and $\hat{p}$. The spectrum of $\hat{x}$ is $[-1;1]$, and the eigenfunctions of $\hat{p}$ are given by the normalised functions $\psi_k(x) = (2a)^{-1/2}\mathrm{e}^{\mathrm{i}kx}$. The boundary conditions imply $\mathrm{e}^{-\mathrm{i}ka} = \mathrm{e}^{\mathrm{i}ka}$ or $2\mathrm{i}ka \in 2\pi\mathrm{i}\mathbb{Z}$, i. e. $k \in \frac{\pi}{a}\mathbb{Z}$, so that the spectrum of $\hat{p}$ is discrete, rather than continuous. Just by changing the domain of definition of the operator, the spectrum changes, even if the commutators stay the same.

We can now summarise a bit: The position and momentum operators, as we have introduced them here, already give us sort of an overview over the mathematical topics of the lecture:

- For $\hat{x}$ there exists a spectrum, where there are no eigenfunctions—in contrast to linear algebra. We therefore need *spectral theory*.
- In physics, one would consider "delta functions" as eigenfunctions of $\hat{x}$; while this is in some sense true (there exists a complete set of generalised eigenfunctions), we at least need to discuss *generalised functions* or *distributions*.
- For $\hat{p}$, we used a derivative. It is, however, not clear, which functions are differentiable, particularly, since we consider L^2 functions, which more precisely are just equvalence classes. We need a more general concept of derivatives, provided by *Sobolev spaces*.

To give a feeling for the fact that these subjects and topics are non-trivial, consider the following exercise.

Exercise 7 (Eigenvalues of hermitian operators)**.**
Consider a hermitian operator A with eigenvector v and eigenvalue λ, i. e. $Av = \lambda v$. Since $\lambda^* \langle v, v\rangle = \langle \lambda v, v\rangle = \langle Av, v\rangle \overset{A\,\text{hermitian}}{=} \langle v, Av\rangle = \langle v, \lambda v\rangle = \lambda \langle v, v\rangle$, the eigenvalue λ must be real.

Now consider $\hat{A} = \hat{x}^3\hat{p} + \hat{p}\hat{x}^3$ and $f(x) := \frac{1}{\sqrt{2}} |x|^{-3/2} \mathrm{e}^{-\frac{1}{4x^2}}$, $x \neq 0$, and $f(0) := 0$. The function f is square-integrable and normalised: $\|f\|_2 = 1$. But $\hat{A}f = \frac{\hbar}{\mathrm{i}} f$. Altogether, $\hat{A}$ is an hermitian operator with an eigenfunction f, but its eigenvalue is not a real number. Where is the error?

2.6 The time-independent Schrödinger equation

Consider a Hamiltonian $\hat{H}$ and the Schrödinger equation $\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\Psi\rangle = \hat{H}|\Psi\rangle$; the formal solution of this is, as already said,

$$|\Psi\rangle_t = U(t)|\Psi\rangle_0, \quad \text{where} \quad U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} \tag{10}$$

How to calculate $U(t)$? If $\hat{H}$ were a matrix (or bounded operator), the power series $\mathrm{e}^x = \sum_{k=0}^{\infty} \frac{x^n}{n!}$ would converge for $x = -\frac{\mathrm{i}}{\hbar}\hat{H}$. For unbounded operators, one has to use the *functional calculus*, which we can explain for hermitian matrices: one diagonalises the matrix, applies the function to every diagonal element separately and then undoes the diagonalisation. Stated otherwise: for a matrix $A = UDU^\dagger$, U unitary and $D = \mathrm{diag}(d_1, \ldots, d_n)$ and a function $f : \mathbb{C} \to \mathbb{C}$ is defined by $f(A) := U\,\mathrm{diag}(f(d_1), \ldots, f(d_n))U^\dagger$. Essentially the same works—as we will see—even for unbounded selfadjoint operator.

In physics, it may happen that $\hat{H}$ is not constant over time, but changes as a function $\hat{H}(t)$. Then the solution $U(t)$ of the *time-dependent Schrödinger*

equation from above does not work. In case $\hat{H}$ is not time-dependent (and has a spectrum of eigenvalues) E_n, we can write $\hat{H} = \sum_{n=0}^{\infty} E_n |n\rangle\langle n|$, where the energies E_n are usually sorted monotically increasing with a lowest value, the *ground state*. Energies belonging to a more-than-one-dimensional subspace are called *degenerate*. This form resembles a diagonal matrix and

$$U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} = \sum_{n=0}^{\infty} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n t} |n\rangle\langle n|. \tag{11}$$

What remains is to find the $|n\rangle$. The eigenvalue equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$ is called the *time-independent Schrödinger equation*. There are a few prominent cases of Hamiltonians where the time-independent Schrödinger equation can be solved: In general, the form of the Hamiltonian in position representation is $\hat{H} = \frac{\vec{p}^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m}\Delta + V(\vec{r})$, where the first part represents the (non-relativistic) kinetic energy $T = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ and V is the potential. Prominent examples are

- the free particle: $V(\vec{r}) = 0$: here the generalised eigenfunctions are $\psi(\vec{r}) \sim \mathrm{e}^{\mathrm{i}\vec{k}\vec{r}}$; this is a plane wave, and this is the reason why states are sometimes called wavefunctions;

- radially symmetric potentials: $V(\vec{r}) = V(r)$ in sperical coordinates with $\vec{r} = r\,(\sin\vartheta\cos\varphi,\, \sin\vartheta\sin\varphi,\, \cos\vartheta)^t$, $r \in \mathbb{R}_0^+$, $\vartheta \in [0;\, \pi]$, $\varphi \in [0;\, 2\pi]$.

  Here, $\Psi(\vec{r}) = \frac{u(r)}{r} Y_{lm}(\vartheta,\, \varphi)$, where $Y_{lm}(\vartheta,\, \varphi)$ are the spherical harmonics (in german: Kugelflächenfunktionen) and u fulfils a radial Schrödinger equation with $V(r) + \frac{l(l+1)\hbar^2}{2mr^2}$ (the second part is a centrifugal potential) on the Hilbert space $L^2(\mathbb{R}_0^+)$, where we require $u(0) = 0$.

- A particular instance of the the Coulomb potential (or hydrogen atom) $V(r) = -\frac{\alpha}{r}$, which gives the basic structure of the periodic table of chemical elements, which will be discussed later in the mathematics part of this lecture.

- Further examples are the harmonic oscillator in three dimensions or the the Woods-Saxon potential $V(r) = \frac{-V_0}{1+\exp(\frac{r-R}{a})}$ and more sophisticated examples from nuclear physics.

There are also other potential like the delta potential $V(x) = -V_0\delta(x)$, also repulsive potentials in scattering theory. Finally, the dimensionality of the problem is often relevant for solutions (in particular, 1D or 3D).

2.6.1 The particle in a box or infinite-well potential

Consider the following potential for a one-dimensional spinless particle:

$$V(x) = \begin{cases} 0 & \text{if } x \in [0;\, L] \\ +\infty & \text{otherwise} \end{cases}. \tag{12}$$

Since outside the range of $[0;\, L]$ the potential is infinite, the state vector must vanish. We require the wavefunction to be continuous, i. e. $\Psi(0) = \Psi(L) = 0$. Essentially the Hilbert space of the system then is $L^2[0;\, L]$, where we must assume appropriate boundary conditions. The solution of such a wave-equation are sine functions $\sin kx$ with appropriate normalisations

$$\psi_k(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi n}{L}\, x\right) \quad \text{with } n \in \mathbb{N}. \tag{13}$$

The energy is $E_n = \frac{\hbar k^2}{2m}$ with $k = 2\pi n/L$ or $E_n = \frac{2\pi^2\hbar}{mL} n^2$. The spectrum is a pure point spectrum $\sim n^2$. There are also other boundary conditions such as periodic boundary conditions (e. g. in solid states), sometimes even periodic up to phase, which give rise to a different spectrum.

Exercise 8 (Boundary conditions)**.**
Consider an inverted parabola (such functions are used in phyics in the Thomas-Fermi theory)

$$\Psi(x) = \sqrt{\frac{30}{L^5}} x(L - x),$$

and calculate the variance $(\Delta H)^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2$*. The first term vanishes, since applying* $\hat{H}^2 = \frac{\hbar^4}{4m^2} \frac{\mathrm{d}^4}{\mathrm{d}x^4}$ *to the parabola gives zero, and* $\langle \hat{H} \rangle^2$ *is positive. Therefore, the variance is negative. Where is the error?*

2.6.2 The harmonic oscillator

One of the most important systems in quantum physics is the *harmonic oscillator*, which is used in various fields in physics; the reason is that in a Taylor expansion a system in the surrounding of a minimum "looks like" a harmonic oscillator locally. Consider an ideal spring with force $F = -Dx$; the associated potential is $V(x) = \frac{1}{2} D x^2$, so that $F = -V'$. Defining an angular frequency by $\omega = \sqrt{D/m}$, we can write a quandratic potential in x as

$$V(x) = \frac{1}{2} m\omega^2 x^2, \tag{14}$$

The Schrödinger equation is then "symmetric" in x and p up to constants, roughly $\sim x^2 + p^2$. Consider the dimensionless operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{\mathrm{i}}{\sqrt{2m\omega\hbar}}\,\hat{p} \qquad \text{and} \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{\mathrm{i}}{\sqrt{2m\omega\hbar}}\,\hat{p}, \tag{15}$$

jointly as ladder operators: $\hat{a}^\dagger$ is the creation, $\hat{a}$ the annihilation operator. It can be seen that $[\hat{a},\, \hat{a}^\dagger] = 1$ (this is equivalent to $[\hat{x},\, \hat{p}] = \mathrm{i}\hbar$), so that these operators are not normal. Define $\hat{n} := \hat{a}^\dagger\hat{a}$ and calculate $[\hat{a},\, \hat{n}] = a]$ and $[\hat{a}^\dagger,\, \hat{n}] = -a^\dagger$. Suppose $\hat{n}\psi = \lambda\psi$; then

$$\hat{n}(\hat{a}\psi) = \hat{a}^\dagger\hat{a}\hat{a}\psi = (\hat{a}\hat{a}^\dagger - 1)\hat{a}\psi = \hat{a}\hat{a}^\dagger\hat{a}\psi - \hat{a}\psi = (\lambda - 1)\hat{a}\psi \tag{16}$$

$$\hat{n}(\hat{a}^\dagger\psi) = \hat{a}^\dagger\hat{a}\hat{a}^\dagger\psi = \hat{a}^\dagger(\hat{a}^\dagger\hat{a} + 1)\psi = \hat{a}^\dagger\hat{a}^\dagger\hat{a}\psi + \hat{a}^\dagger\psi = (\lambda + 1)\hat{a}^\dagger\psi \tag{17}$$

That is, once we have found an eigenfunction of $\hat{n}$ we get a whole sequence of eigenfunctions with eigenvalues shifted by an integer. We should check the normalisation of $\hat{a}\psi$ and $\hat{a}^\dagger\psi$, if ψ is an eigenvector of $\hat{n}$ with eigenvalue λ: there hold $\langle\hat{a}^\dagger\psi|\hat{a}^\dagger\psi\rangle = \langle\psi|\hat{a}\hat{a}^\dagger\psi\rangle = \lambda + 1$ and $\langle\hat{a}\psi|\hat{a}\psi\rangle = \langle\psi|\hat{a}^\dagger\hat{a}\psi\rangle = \lambda$.

Now due to $\langle\psi|\hat{n}\psi\rangle = \langle\hat{a}\psi|\hat{a}\psi\rangle \geq 0$, the operator $\hat{n}$ is positive semidefinite, and $\lambda \geq 0$. We find a *ground state*, a normalised Gaussian

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{18}$$

with eigenvalue $\lambda = 0$ and note that $\hat{a}\psi_0$ is the null vector, which cannot be normalised. On the other hand, by applying $\hat{a}^\dagger$ repeatedly on ψ_0, we find eigenstates with eigenvalues $n \in \mathbb{N}_0$. This is the infinite sequence of so-called Fock states $|0\rangle$, $|1\rangle$, $|2\rangle$, … with energies $E_n = \hbar\omega(n + 1/2)$ in an infinite-dimensional Hilbert space. The state $|0\rangle$ is called the ground state (or vacuum state, if n counts photons etc.), the infinite sequence $|n\rangle$, $n \in \mathbb{N}$ are the (normalised) excited states defined by $|n+1\rangle := \frac{\hat{a}^\dagger|n\rangle}{\sqrt{n+1}}$.

Since the eigenvalues of $\hat{n}$ must not be negative, we can exclude the existence of eigenvectors with non-integer eigenvalues. Moreover, it can be shown that the Fock states form an orthonormal basis of the Hilbert space $L^2(\mathbb{R})$, and the spectrum of the harmonic oscillator is a pure point spectrum. We can thus write an arbitrary state in the form

$$|\Psi\rangle = \sum\nolimits_{n=0}^{\infty} a_n\,|n\rangle, \tag{19}$$

where $a = (a_n)_{n\in\mathbb{N}_0} = (a_0,\, a_1,\, a_2,\, a_3,\, \dots) \in \mathbb{C}^{\mathbb{N}_0}$ is a square-normalised sequence of complex numbers, i. e. $\sum_{n=0}^{\infty} |a_n|^2 = 1$. In view of this, every vector $|\Psi\rangle$ can uniquely be identified with a sequence a in the Hilbert space

$\ell^2(\mathbb{N}_0)$, which by construction is separable. The identification (an isomorphism) shows the separability of the Hilbert space $L^2(\mathbb{R})$, and the same holds for $L^2(\mathbb{R}^n)$.

In mathematics, there is commonly used an isometric (right) shift operator $\hat{s}$, and its inverse $\hat{s}^\dagger$ on $\ell^2(\mathbb{N}_0)$ defined by

$$\hat{s} = \sum_{n=0}^{\infty} |n+1\rangle\langle n| : \quad (a_0,\, a_1,\, a_2,\, a_3,\, \dots) \mapsto (0,\, a_0,\, a_1,\, a_2,\, \dots) \tag{20}$$

$$\hat{s}^\dagger = \sum_{n=0}^{\infty} |n\rangle\langle n+1| : \quad (a_0,\, a_1,\, a_2,\, a_3,\, \dots) \mapsto (a_1,\, a_2,\, a_3,\, a_4,\, \dots) \tag{21}$$

Note that $\hat{s}^\dagger\hat{s} = \mathbb{1}$ with spectrum $\{1\}$, while $\hat{s}\hat{s}^\dagger = \mathbb{1} - |0\rangle\langle 0|$ is a projector with spectrum $\{0,\, 1\}$. (Usually for bounded operators, the spectrum of AB and BA is the same up to possible zeros.) Using the square root of the number operator, $\sqrt{\hat{n}} = \sum_{n=0}^{\infty} \sqrt{n}|n\rangle\langle n|$ or $(a_0,\, a_1,\, a_2,\, a_3,\, \dots) \mapsto (0,\, a_1,\, \sqrt{2}a_2,\, \sqrt{3}a_3,\, \dots)$, we can write

$$\hat{a} = \sum_{n=0}^{\infty} \sqrt{n+1}|n\rangle\langle n+1| = \hat{s}^\dagger\sqrt{\hat{n}} \tag{22}$$

$$\hat{a}^\dagger = \sum_{n=0}^{\infty} \sqrt{n+1}|n+1\rangle\langle n| = \sqrt{\hat{n}}\hat{s} \tag{23}$$

Here the operators are decomposed into what is called a *polar decomposition*, where $\hat{s}$ and $\hat{s}^\dagger$ are partial isometries.

2.7 Playing around with operators

As an example, we shall calculate for the states $|n\rangle$ uncertainties of position and momentum $(\Delta x)^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$ and $(\Delta p)^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2$. We rewrite $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^\dagger)$ and $\hat{p} = -\mathrm{i}\sqrt{\frac{m\omega\hbar}{2}}\,(\hat{a} - \hat{a}^\dagger)$ and immediately see that $\langle\hat{x}\rangle^2 = \langle\hat{p}\rangle^2 = 0$ due to $\langle n|\hat{a}|n\rangle = \langle n|\hat{a}^\dagger|n\rangle = 0$. In the expansions of $\hat{x}^2$ and $\hat{p}^2$ the non-vanishing terms of $(\hat{a}^\dagger \pm \hat{a}^\dagger)^2$ are $\pm(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) = \pm(2\hat{n}+1)$. Therefore,

$$(\Delta\hat{x})^2 = \frac{\hbar}{2m\omega}\cdot(2n+1) \quad \text{and} \quad (\Delta\hat{p})^2 = \frac{m\omega\hbar}{2}\cdot(2n+1) \tag{24}$$

and $\Delta\hat{x}\Delta\hat{p} = (n+\frac{1}{2})\hbar$. So of the Fock states, only the ground state has minimum uncertainty. To find other states with minimum uncertainty, we need some formulae.

Lemma 9 (Baker-Campbell-Hausdorff (BCH) and related formulae)**.**
For (bounded) operators $A,\, B \in \mathcal{B}(\mathcal{H})$ there holds (by Taylor expansion)

$$\mathrm{e}^{tA}B\mathrm{e}^{-tA} = B + t[A,\, B] + \frac{t^2}{2!}[A,\, [A,\, B]] + \frac{t^3}{3!}[A,\, [A,\, [A,\, B]]] + \dots$$

Furthermore, if $[A,\, [A,\, B]] = [B,\, [A,\, B]] = 0$, there holds the Zassenhaus formula

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-\frac{1}{2}[A,\, B]}.$$

We will nevertheless apply these formulae to unbounded operators and do not worry about domains of definition. We can define so-called unitary *displacement operators*

$$\hat{D}(\alpha) := \mathrm{e}^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = \mathrm{e}^{\mathrm{i}\left(\mathrm{Im}\,\alpha\cdot\sqrt{\frac{2m\omega}{\hbar}}\,\hat{x} - \mathrm{Re}\,\alpha\cdot\sqrt{\frac{2}{m\omega\hbar}}\,\hat{p}\right)} \quad \text{for } \alpha \in \mathbb{C} \tag{25}$$

Using $[\alpha\hat{a}^\dagger - \alpha^*\hat{a},\, \beta\hat{a}^\dagger - \beta^*\hat{a}] = -\alpha\beta^*[\hat{a}^\dagger,\, \hat{a}] - \alpha^*\beta[\hat{a},\, \hat{a}^\dagger] = \alpha\beta^* - \alpha^*\beta$, we calculate

$$\hat{D}(\alpha+\beta) = \mathrm{e}^{(\alpha\hat{a}^\dagger - \alpha^*\hat{a}) + (\beta\hat{a}^\dagger - \beta^*\hat{a})} = \hat{D}(\alpha)\hat{D}(\beta)\mathrm{e}^{\frac{\alpha^*\beta - \alpha\beta^*}{2}} \tag{26}$$

or $\hat{D}(\beta)\hat{D}(\alpha) = \hat{D}(\alpha)\hat{D}(\beta)\mathrm{e}^{\alpha^*\beta - \alpha\beta^*}$, i. e. the displacement "commute up to a phase" and thus are a projective representation of $\mathbb{C}$. In particular, $\hat{D}(0) = \mathbb{1}$ and $\hat{D}(\alpha)^{-1} = \hat{D}(\alpha)^\dagger = \hat{D}(-\alpha)$.

It is easy to see that $\hat{a}^\dagger$ does not have any eigenvalue, since $\hat{a}^\dagger|\Psi\rangle$ has a zero vacuum component. However, for every $\alpha \in \mathbb{C}$, $\hat{a}$ possesses an eigenfunction $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$. In lemma 9, let $A = -(\alpha\hat{a}^\dagger - \alpha^*\hat{a})$ and $B = \hat{a}$, so that $\hat{D}(-\alpha)\hat{a}\hat{D}(\alpha) = \hat{a} + \alpha$; therefore,

$$\hat{a}\hat{D}(\alpha)|0\rangle = \hat{D}(\alpha)(\hat{a}+\alpha)|0\rangle = \alpha\hat{D}(\alpha)|0\rangle. \tag{27}$$

Explicitely, the *coherent states* $|\alpha\rangle$ read $|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$, which all have minimum uncertainty $\Delta x\Delta p = \hbar/2$. There are also other minimum uncertainty states, the *squeezed states*, where e. g. $\Delta\hat{x} \sim \Delta\hat{p}^{-1}$.

2.8 The Stone-von-Neumann theorem

We have already found that the Heisenberg commutators $[\hat{x}_i,\, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}$ do not uniquely determine the spectrum of the operators by considering them on different domains such as $\mathbb{R}$ and $[a;\, b]$. Intuitively this can be understood by noting that this relation holds locally, in the neighbourhood of a point $x \in \mathbb{R}^n$. Therefore, to get uniqueness, we need to use operators with "global" properties. To this aim, we use the following statement.

Lemma 10 (Unitary one-parameter groups)**.**
Let A be a (possibly unbounded) self-adjoint operator on $\mathcal{H}$ and let $U(t) := \mathrm{e}^{iAt}$ for $t \in \mathbb{R}$ (e. g. the time evolution of a Hamiltonian). Then,

1. *for every $t \in \mathbb{R}$, $U(t)$ is unitary, and $U(t+s) = U(t)U(s)$ (one-parameter group) and*
2. *for every $\psi \in \mathcal{H}$ and $t \to t_0$, $U(t)\psi \to U(t_0)\psi$ (strong continuity),*

i. e. $U(t)$ is a strongly continuous unitary one-parameter group. Stone's theorem tells us that every strongly continuous unitary one-parameter group has a generator like A, which can be found by "differentiating".

Now consider the *translations* in position space by $[U(a)\Psi](x) := \Psi(x + a)$ (a shift to the left), which form a unitary strongly continuous unitary one-parameter group, and we want to know the generator A. We formally calculate for every $x \in \mathbb{R}$ and some Ψ in the domain of definition,

$$\frac{\mathrm{d}U}{\mathrm{d}a}(a_0)\Psi(x) = \lim_{h\to 0} \frac{U(a_0+h) - U(a_0)}{h}\Psi(x) \tag{28}$$

$$= \lim_{h\to 0} \frac{\Psi(x+a_0+h) - \Psi(x+a_0)}{h} = \frac{\mathrm{d}\Psi}{\mathrm{d}x}(x+a_0), \tag{29}$$

and, in particular $\frac{\mathrm{d}U}{\mathrm{d}a}(0) = \frac{\mathrm{d}}{\mathrm{d}x}$ pointwise. Comparing with $\frac{\mathrm{d}U}{\mathrm{d}a}(a) = \mathrm{i}AU(a)$ and setting $a = 0$, we have $A = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\hat{p}}{\hbar}$, i. e. $U(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}a\hat{p}}$. Thus, in physics terms, the momentum is the generator of translations in position, and the same holds vice versa: the position is the generator of translations in momentum. By this we see that we can distinguish $\hat{p}$ on $\mathbb{R}$ and on $[a; b]$ (free particle vs. infinite-well potential), since in the former case we would "hit the wall". We shall thus use exponentiated operators to find a certain uniqueness.

Applying lemma 9 to the (unbounded!) A and B with $[A, B] = \mathrm{i}\hbar$ we find

$$\mathrm{e}^{\mathrm{i}(sA+tB)} = \mathrm{e}^{-\frac{\mathrm{i}^2 st}{2}[A,B]}\mathrm{e}^{\mathrm{i}sA}\mathrm{e}^{\mathrm{i}tB} = \mathrm{e}^{-\frac{\mathrm{i}^2 st}{2}[B,A]}\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{\mathrm{i}sA} \tag{30}$$

$$= \mathrm{e}^{\frac{\mathrm{i}st\hbar}{2}}\mathrm{e}^{\mathrm{i}sA}\mathrm{e}^{\mathrm{i}tB} = \mathrm{e}^{\frac{-\mathrm{i}st\hbar}{2}}\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{\mathrm{i}sA} \tag{31}$$

or $\mathrm{e}^{\mathrm{i}sA}\mathrm{e}^{\mathrm{i}tB} = \mathrm{e}^{-\mathrm{i}st\hbar}\mathrm{e}^{\mathrm{i}tB}\mathrm{e}^{\mathrm{i}sA}$ or the Weyl commutator relations (this is a group-theoretic commutator rather than the usual algebraic commutators.) We now formulate the uniqueness theorem.

Theorem 11 (Stone-von Neumann theorem)**.**
Let $i, j \in \{1, \ldots, n\}$ and consider operators A_i and B_j on a Hilbert space $\mathcal{H}$, such that the following Weyl *commutator relations are fulfilled:*

$$\mathrm{e}^{\mathrm{i}tA_i}\mathrm{e}^{\mathrm{i}sA_j} = \mathrm{e}^{\mathrm{i}sA_j}\mathrm{e}^{\mathrm{i}tA_i}$$
$$\mathrm{e}^{\mathrm{i}tB_i}\mathrm{e}^{\mathrm{i}sB_j} = \mathrm{e}^{\mathrm{i}sB_j}\mathrm{e}^{\mathrm{i}tB_i}$$
$$\mathrm{e}^{\mathrm{i}tA_i}\mathrm{e}^{\mathrm{i}sB_j} = \mathrm{e}^{-\mathrm{i}st\delta_{ij}}\mathrm{e}^{\mathrm{i}sB_j}\mathrm{e}^{\mathrm{i}tA_i}$$

Suppose that the operators act irreducibly on $\mathcal{H}$, i. e. $\{0\}$ und $\mathcal{H}$ are closed subspaces invariant with respect to all $\mathrm{e}^{\mathrm{i}tA_i}$ und $\mathrm{e}^{\mathrm{i}tB_i}$ (otherwise, the theorem

can be adapted). Then, there exist unitary operator $U : \mathcal{H} \to L^2(\mathbb{R}^n)$*, which is unique up to a phase* $\mathrm{e}^{\mathrm{i}\varphi}$*, such that*

$$U\mathrm{e}^{\mathrm{i}tA_i}U^{-1} = \mathrm{e}^{\mathrm{i}t\hat{x}_i} \quad \textit{and} \quad U\mathrm{e}^{\mathrm{i}tB_i}U^{-1} = \mathrm{e}^{\mathrm{i}t\hat{p}_i}.$$

The intuitive reason behind this is that the Heisenberg operators exhibit the local properties (at one point x), but not the global ones. The Weyl commutators take into account global properties; remember that the exponentiated operators are translations of momentum and position, respectively. (This is related to the theory of Lie groups and Lie algebras.)

We can only sketch the proof here. First, the irreducibility is needed. Consider the Hilbert space $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ and operators $\hat{x} = x \oplus x$ and $\hat{p} = \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x} \oplus \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}$. These operators fulfil the canonical commutation relations, but $\mathcal{H}' = \{f \oplus f \,|\, f \in L^2(\mathbb{R})\}$ is an invariant subspace.

We define a bounded operator (the Weyl quantisation, see next section)

$$Q(f) = (2\pi)^{-n} \int_{\vec{a},\vec{b}\in\mathbb{R}^n} (\mathfrak{F}f)(\vec{a},\,\vec{b})\, \mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}\, \mathrm{d}^n\vec{a}\, \mathrm{d}^n\vec{b}, \tag{32}$$

where $(\mathfrak{F}f)(\vec{a},\vec{b}) = (2\pi)^{-n} \int_{\vec{x},\vec{p}\in\mathbb{R}^n} f(\vec{x},\vec{p})\mathrm{e}^{-\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}\, \mathrm{d}^n\vec{x}\, \mathrm{d}^n\vec{p}$ is the Fourier transform of f. Choosing $f_0(\vec{x},\vec{p}) := 2^n\mathrm{e}^{-\frac{|\vec{x}|^2}{\sigma}}\mathrm{e}^{-\sigma\frac{|\vec{p}|^2}{\hbar^2}}$, we have some remarkable properties, namely for every $\vec{a},\,\vec{b} \in \mathbb{R}^n$ there holds

$$Q(f_0)\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{A}}+\vec{b}\cdot\hat{\vec{B}})}Q(f_0) = \mathrm{e}^{\frac{-\sigma|\vec{a}|^2}{4}}\mathrm{e}^{-\frac{\hbar^2|\vec{b}|^2}{4\sigma}}Q(f_0). \tag{33}$$

In particular, the right-hand side does not depend on $\hat{\vec{A}}$ and $\hat{\vec{B}}$. Moreover, since f_0 is real-valued, $Q(f_0)$ is self-adjoint and thus an orthogonal projection. Now, let $\mathcal{H}' := Q(f_0)\mathcal{H}$ be the image of this projection (which is non-zero), and choose $\varphi,\,\psi \in \mathcal{H}'$. Then,

$$\begin{aligned}
\langle \mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{A}}+\vec{b}\cdot\hat{\vec{B}})}\varphi | \mathrm{e}^{\mathrm{i}(\vec{a}'\cdot\hat{\vec{A}}+\vec{b}'\cdot\hat{\vec{B}})}\psi\rangle &= \langle Q(f_0)\varphi | \mathrm{e}^{-\mathrm{i}(\vec{a}\cdot\hat{\vec{A}}+\vec{b}\cdot\hat{\vec{B}})}\mathrm{e}^{\mathrm{i}(\vec{a}'\cdot\hat{\vec{A}}+\vec{b}'\cdot\hat{\vec{B}})}Q(f_0)\psi\rangle \\
&= \mathrm{e}^{\frac{\mathrm{i}\hbar(\vec{a}\cdot\vec{b}')-\vec{b}\cdot\vec{a}')}{2}}\langle\varphi|Q(f_0)\mathrm{e}^{\mathrm{i}((\vec{a}'-\vec{a})\cdot\hat{\vec{A}}+(\vec{b}'-\vec{b})\cdot\hat{\vec{B}})}Q(f_0)\psi\rangle \\
&= \mathrm{e}^{\frac{\mathrm{i}\hbar(\vec{a}\cdot\vec{b}')-\vec{b}\cdot\vec{a}')}{2}}\mathrm{e}^{\frac{-\sigma|\vec{a}'-\vec{a}|^2}{4}}\mathrm{e}^{-\frac{\hbar^2|\vec{b}'-\vec{b}|^2}{4\sigma}}\langle\varphi|\psi\rangle.
\end{aligned}$$

Again, the overlap depends only on $\vec{a}$ and $\vec{b}$ and not on the explicit forms of $\hat{\vec{A}}$ and $\hat{\vec{B}}$, from which we used only their commutator relations. The essence of the proof is that we can replace in this formula A_i by $\hat{x}_i$ and B_i by $\hat{p}_i$ without changing inner products. We therefore have to identify vectors in the Hilbert space $\mathcal{H}$ with vectors in $L^2(\mathbb{R}^n)$.

3 Quantisation

Up to now, we have discussed self-adjoint operators of position and momentum and spin. Apart from quantities, for which there exists no classical analog, we would like to start with a classial observable and "quantise" it, i. e. to find a corresponding self-adjoint operator.

3.1 Weyl quantisation

We have seen that position and momentum are the defining variables for a classical physical system. We also know what their quantum-mechanical counterparts are, the operators $\hat{x}$ and $\hat{p}$ with $[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar$. How to quantise an arbitrary function $f(\vec{x}, \vec{p})$? The standard Hamilton operator we simply get by formally replacing $\hat{x}$ and $\hat{p}$ by their operators in the Hamiltonian function. For other quantities, e. g. for xp, this is not so simple: should we quantise it as $\hat{x}\hat{p}$, as $\hat{p}\hat{x}$ or as something else? Here enters the so-called *operator ordering*; our quantum-mechanical operators should be selfadjoint, so at least they should formally be hermitian. A solution to this question is given by the Weyl ordering and the Weyl quantisation; there are other important orderings such as normal ordering which we shall not treat here.[2]

Given a monomial $x^{n-k}p^k$ of order $n \in \mathbb{N}_0$, we set its Weyl quantisation Q_W to be the totally symmetric homogeneous polynomial of n-th order

$$Q_W(x^{n-k}p^k) := \frac{1}{n!} \sum_{\sigma \in S_n} \sigma(\underbrace{\hat{x}, \ldots, \hat{x}}_{n-k\,\text{times}}, \underbrace{\hat{p}, \ldots, \hat{p}}_{k\,\text{times}}), \tag{34}$$

where $\sigma(A_1, \ldots, A_n) = A_{\sigma_1} \ldots A_{\sigma_n}$ is a permutation of the operators and S_n the symmetric group consisting of all $n!$ of the numbers $\{1, \ldots, n\}$. This concept also works for systems with more $\hat{x}_i$ and $\hat{p}_j$, since the operators for different i and j commute. The Weyl quantisation can be uniquely characterised by the property that

$$Q_W((ax + bp)^k) = (a\hat{x} + b\hat{p})^k \tag{35}$$

for all $k \in \mathbb{N}_0$ and $a, b \in \mathbb{C}$. Extending this to more than one variable $\mathbb{R}^{2n}$, and formally applying a power series results in

$$Q_W(\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\vec{x} + \vec{b}\cdot\vec{p})}) = \mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}} + \vec{b}\cdot\hat{\vec{p}})} \tag{36}$$

The basic idea now is to express an arbitrary function $f(\vec{x}, \vec{p})$ as the inverse fourier transform of its fourier transform $\mathfrak{F}f$ by

$$f(\vec{x}, \vec{p}) = \frac{1}{(2\pi)^n} \int_{(\vec{a}, \vec{b}) \in \mathbb{R}^{2n}} (\mathfrak{F}f)(\vec{a}, \vec{b})\, \mathrm{e}^{\mathrm{i}(\vec{a}\cdot\vec{x} + \vec{b}\cdot\vec{p})}\, \mathrm{d}^{2n}(\vec{a}, \vec{b}) \tag{37}$$

[2] Note again that a simple symmetrisation need not always work as the exercise 7 shows.

and to replace the exponential by its Weyl quantisation as in eq. (36).[3] The right hand side is then defined to be $Q_W(f)$ and is an operator acting on $L^2(\mathbb{R}^n)$. To determine the action of the operators $\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}$ consider for every $\vec{a},\,\vec{b}\in\mathbb{R}^n$ the (stronly continuous unitary one-parameter) group

$$(U_{\vec{a},\,\vec{b}}(t)\psi)(\vec{x}) := \mathrm{e}^{\frac{\mathrm{i}t^2\hbar(\vec{a},\,\vec{b})}{2}}\mathrm{e}^{\mathrm{i}t\vec{a}\cdot\hat{\vec{x}}}\psi(\vec{x}+t\hbar\vec{b}). \tag{38}$$

By doing a formal derivative we find that this group is generated by $\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}}$.[4] We know that momentum is a generator of translations in space, $(\mathrm{e}^{\mathrm{i}t\vec{b}\cdot\hat{\vec{p}}}\psi)(\vec{x}) := \psi(\vec{x}+t\hbar\vec{b})$, so that we can write

$$\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})} = \mathrm{e}^{\frac{\mathrm{i}t^2\hbar(\vec{a},\,\vec{b})}{2}}\mathrm{e}^{\mathrm{i}t\vec{a}\cdot\hat{\vec{x}}}\mathrm{e}^{\mathrm{i}t\vec{b}\cdot\hat{\vec{p}}} \tag{39}$$

without having to invoke the BCH formula here. We shall now write $\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}$ in terms of a kernel operator k, i. e.

$$(\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}\psi)(\vec{x}) = \int_{y\in\mathbb{R}^n} k(\vec{x},\,\vec{y})\psi(\vec{y})\,\mathrm{d}^n\vec{y} \tag{40}$$

with $k(\vec{x},\,\vec{y}) = \mathrm{e}^{\frac{\mathrm{i}\hbar(\vec{a},\,\vec{b})}{2}}\mathrm{e}^{\mathrm{i}\vec{a}\cdot\hat{\vec{x}}}\delta(\vec{x}+\hbar\vec{b}-\vec{y})$, where we use the n-dimensional delta function. We can rewrite this expression by

$$\begin{aligned}(Q_W(f)\psi)(y) &= (2\pi)^{-n}\int_{(\vec{a},\,\vec{b})\in\mathbb{R}^{2n}}(\mathfrak{F}f)(\vec{a},\,\vec{b})\left[\int_{x\in\mathbb{R}^n}k(\vec{x},\,\vec{y})\psi(\vec{y})\,\mathrm{d}^n\vec{y}\right]\,\mathrm{d}^{2n}(\vec{a},\,\vec{b})\\ &= \int_{y\in\mathbb{R}^n}k_f(\vec{x},\,\vec{y})\psi(\vec{y})\,\mathrm{d}^n\vec{y}.\end{aligned}$$

We use $\int_{x\in\mathbb{R}^n}\mathrm{e}^{\pm\mathrm{i}a(\vec{x}-\vec{x_0})}\,\mathrm{d}^n\vec{x} = (\frac{2\pi}{a})^n\delta(\vec{x}-\vec{x_0})$ to find

$$\begin{aligned}k_f(\vec{x},\,\vec{y}) &:= (2\pi)^{-n}\int_{(\vec{a},\,\vec{b})\in\mathbb{R}^{2n}}(\mathfrak{F}f)(\vec{a},\,\vec{b})\mathrm{e}^{\frac{\mathrm{i}\hbar(\vec{a},\,\vec{b})}{2}}\mathrm{e}^{\mathrm{i}\vec{a}\cdot\hat{\vec{x}}}\delta(\vec{x}+\hbar\vec{b}-\vec{y})\,\mathrm{d}^{2n}(\vec{a},\,\vec{b})\\ &\overset{\vec{b}':=\hbar\vec{b}}{=}(2\pi\hbar)^{-n}\int_{(\vec{a},\,\vec{b}')\in\mathbb{R}^{2n}}(\mathfrak{F}f)\left(\vec{a},\,\frac{\vec{b}'}{\hbar}\right)\mathrm{e}^{\frac{\mathrm{i}(\vec{a},\,\vec{b}')}{2}}\mathrm{e}^{\mathrm{i}\vec{a}\cdot\hat{\vec{x}}}\delta(\vec{x}+\vec{b}'-\vec{y})\,\mathrm{d}^{2n}(\vec{a},\,\vec{b}')\\ &= (2\pi\hbar)^{-n}\int_{\vec{a}\in\mathbb{R}^n}(\mathfrak{F}f)\left(\vec{a},\,\frac{\vec{y}-\vec{x}}{\hbar}\right)\mathrm{e}^{\frac{\mathrm{i}\vec{a}(\vec{x}+\vec{y})}{2}}\,\mathrm{d}^n\vec{a}.\end{aligned}$$

The last term is (up to a constant) the partial inverse Fourier transform with respect to the second component at the point $(\frac{\vec{x}+\vec{y}}{2},\,\frac{\vec{y}-\vec{x}}{\hbar})$. So we may

[3] We do not formally introduce integrals of operators.

[4] Doing the derivative of the right-hand side gives the prefactor $\mathrm{i}\hbar t\vec{a},\,\vec{b}+\mathrm{i}\vec{a}\cdot\hat{\vec{x}}+\mathrm{i}\vec{a}\cdot\hat{\vec{p}}$ to the exponential function; the first term vanishes, the third is precisely the same as we did it before.

as well take the original function f and transform it with respect to the first component, so that

$$k_f(\vec{x},\,\vec{y}) := (2\pi\hbar)^{-n} \int_{\vec{p}\in\mathbb{R}^n} f\left(\frac{\vec{x}+\vec{y}}{2},\,\vec{p}\right) \mathrm{e}^{-\frac{\mathrm{i}\vec{p}(\vec{y}-\vec{x})}{\hbar}}\;\mathrm{d}^n\vec{p}.$$

Strictly speaking, this expression needs not to be convergent, but can be understood pointwise. The operator $\hat{A}$ is the operator belonging to this kernel; in physics notation one would write with

$$Q_W(f) = \int_{(\vec{x},\,\vec{y})\in\mathbb{R}^{2n}} k_f(\vec{x},\,\vec{y})\,|\vec{x}\rangle\langle\vec{y}|\,\mathrm{d}^{2n}(\vec{x},\,\vec{y}),$$

where $|\vec{x}\rangle\langle\vec{y}|$ is strictly speaking not defined everywhere. This process can be done for functions on the phase space $L^2(\mathbb{R}^n\times\mathbb{R}^n)$ and results in a bounded operator, more precisely a Hilbert-Schmidt operator; note that polynomials with which we started are in usually not L^2 functions.

3.2 Trace of operators and compact operators

In linear algebra, the trace of an operator is the sum of its diagonal elements. By the commutativity $\operatorname{Tr} AB = \operatorname{Tr} BA$, the trace is invariant with respect to a basis change $A \mapsto UAU^{-1}$. We can generalise this notion to some operators $\mathcal{B}(\mathcal{H})$ on a Hilbert space by setting $\operatorname{Tr} A := \sum_{i\in I}\langle i|A|i\rangle$, where the $|i\rangle$ form an orthonormal basis of $\mathcal{H}$. Now we sum up possibly an infinite amount of complex numbers $\langle i|A|i\rangle$, and at this point we cannot say anything about the convergence of such sum. However, if we take A to be a positive operator (in a separable Hilbert space), $\langle i|A|i\rangle \geq 0$, and either the series is absolutely convergent or diverges to infinity.

Now, for any $A\in\mathcal{B}(\mathcal{H})$, the operator $A^\dagger A$ is positive, and we can define its square root by $|A| := \sqrt{A^\dagger A}$, so that the spectrum is contained in $\mathbb{R}_0^+$. If the trace should exist at all, the spectrum of $|A|$ (the singular values of A) must be given by a null sequence. It is then a compact operator on $\mathcal{H}$, which in this case is the uniform limit of operators with finite rank. Therefore, they behave somewhat like matrices. Similar to the usual p-norms in functional analysis, we can define

$$\|A\|_p := [\operatorname{Tr}(|A|^p)]^{1/p} \tag{41}$$

for $p\in(1;\,\infty)$, provided, $\operatorname{Tr}|A|^p$ is finite. In particular, for $p=1$ we get trace-class operators (such as the density operator), for $p=2$ Hilbert-Schmidt operators. (For $p=\infty$ we get the non-compact bounded operators.) There holds the following theorem, which is relevant for the quantisation scheme.

Theorem 12 (Hilbert-Schmidt operators)**.**
Let (Ω, Σ, μ) *be a measure space and* $\mathcal{H} := L^2(\Omega)$*. An operator* $A \in \mathcal{B}(\mathcal{H})$ *is a Hilbert-Schmidt operator, if and only if there exists a function* $f \in L^2(\Omega \times \Omega)$*, such that*

$$(Af)(x) = \int_{y\in\Omega} k(x, y) f(y) \mathrm{d}\mu(y),$$

and in this case, there holds $\|A\|_2 = \|k\|_2 := \left(\int_{x,\, y\in\Omega} |k(x, y)|^2 \, \mathrm{d}x \, \mathrm{d}y\right)^{1/2}$.

We do not give a proof here, but for the norm equalities compare the case of matrices, i. e. $\Omega = \{1, \ldots, n\}$ with the counting measure. Then, for $A = (a_{ij})_{i,j=1}^n$, we compute $\|A\|_2^2 = \sum_{i,j=1}^n |a_{ij}|^2$ and similarly for k.

3.3 Dequantisation and the Wigner function

The quantisation map Q_W possesses an inverse, a *dequantisation*.

Theorem 13 (Dequantisation)**.**
The map Q_W *is unitary up to a constant from* $L^2(\mathbb{R}^{2n})$ *to the Hilbert-Schmidt operators on* $\mathcal{H} = L^2(\mathbb{R}^n)$ *with inverse*

$$[Q_W^{-1}(A)](\vec{x}, \vec{p}) = \hbar^n \int_{\vec{b}\in\mathbb{R}^n} k\left(\vec{x} - \frac{\hbar\vec{b}}{2}, \vec{x} + \frac{\hbar\vec{b}}{2}\right) \mathrm{e}^{\mathrm{i}\vec{b}\cdot\vec{p}} \, \mathrm{d}\vec{b}. \tag{42}$$

Further, $Q_W(f^*) = Q_W(f)^\dagger$*, and* $Q_W(f)$ *is selfadjoint, if and only if* f *is real-valued. (Note that the adjoint of an operator given by* $k(x, y)$ *is given by* $k(y, x)^*$*, similarly as for matrices.)*

Up to now we have quantised classical phase-space functions. The inverse mapping now also allows us to dequantise genuinely quantum-mechanical operators, in particular the density operator ρ, since this is of trace class and thus Hilbert-Schmidt. The dequantisation of ρ is known as the Wigner function $W_\rho(\vec{x}, \vec{p})$, and we have two equivalent formulations of quantum mechanics. We required that ρ is trace-normalised, which is translated to $\int W = 1$; however, it is not clear, which phase-space functions correspond to positive semidefinite operators (although there are restrictions on the functions).

Now classically a state would be a probability distribution P on the phase space (a pure state a point-distribution) and we can express expectation values by $\langle f \rangle = \int_{\vec{x},\vec{p}\in\mathbb{R}^{2n}} P(\vec{x}, \vec{p}) f(\vec{x}, \vec{p}) \mathrm{d}^{2n}(\vec{x}, \vec{p})$. Usually we quantise f and calculate expectation values in Hilbert space by a density operator ρ. But we could also dequantise the density operator to the Wigner function $W(\vec{x}, \vec{p})$ and calculate expectation values in phase space. But note, in particular, that not every probability distribution corresponds to a Wigner function (we can violate the uncertainty principle by a point distribution) and that unlike classical probability distributions Wigner functions may have negative parts.

3.4 The Moyal star product

We have seen that there are two different ways of discussing quantum mechanics. The bounded operators (and some of their subclasses) on a Hilbert space form an algebra, i. e., they can be multiplied. In particular, the product of two Hilbert-Schmidt operators is—by Cauchy-Schwarz—trace-class and thus again a Hilbert-Schmidt operator. Therefore, given $Q_W(f)$ and $Q_W(g)$, there exists a function $Q_W(f * g)$, such that $Q_W(f)Q_W(g) = Q_W(f * g)$. To calculate this functions we invoke the original quantisation formula

$$Q_W(f)Q_W(g) = (2\pi)^{-2n} \int_{\vec{a},\vec{b},\vec{a}',\vec{b}'\in\mathbb{R}} (\mathfrak{F}f)(\vec{a},\vec{b})(\mathfrak{F}g)(\vec{a}',\vec{b}')\, \mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}\, \mathrm{e}^{\mathrm{i}(\vec{a}'\cdot\hat{\vec{x}}+\vec{b}'\cdot\hat{\vec{p}})}\, \mathrm{d}^{4n}(\vec{a},\vec{b},\vec{a}',\vec{b}')$$

Using $\mathrm{e}^{\mathrm{i}(\vec{a}\cdot\hat{\vec{x}}+\vec{b}\cdot\hat{\vec{p}})}\, \mathrm{e}^{\mathrm{i}(\vec{a}'\cdot\hat{\vec{x}}+\vec{b}'\cdot\hat{\vec{p}})} = \mathrm{e}^{-\mathrm{i}\hbar\frac{\vec{a}\vec{b}'-\vec{b}\vec{a}'}{2}} \mathrm{e}^{\mathrm{i}((\vec{a}+\vec{a}')\cdot\hat{\vec{x}}+(\vec{b}+\vec{b}')\cdot\hat{\vec{p}})}$, substituting $\vec{a}$ by $\vec{a}''-\vec{a}'$ and $\vec{a}$ by $\vec{b}''-\vec{b}'$ and using $\vec{a}\vec{b}'-\vec{b}\vec{a}' = \vec{a}''\vec{b}'-\vec{b}''\vec{a}'$, this may be rewritten as

$$Q_W(f)Q_W(g) = (2\pi)^{-n} \int_{\vec{a}'',\vec{b}''\in\mathbb{R}} [\mathfrak{F}(f*g)](\vec{a}'',\vec{b}'')\, \mathrm{e}^{\mathrm{i}(\vec{a}''\cdot\hat{\vec{x}}+\vec{b}''\cdot\hat{\vec{p}})}\, \mathrm{d}^{2n}(\vec{a}'',\vec{b}''),$$

which is the quantisation of the function $f * g$ with

$$\begin{aligned}[\mathfrak{F}(f*g)](\vec{a},\vec{b}) = (2\pi)^{-n} \int_{\vec{a}',\vec{b}'\in\mathbb{R}} & \mathrm{e}^{-\mathrm{i}\hbar\frac{\vec{a}\vec{b}'-\vec{b}\vec{a}'}{2}} \\ & \times (\mathfrak{F}f)(\vec{a}-\vec{a}',\vec{b}-\vec{b}')(\mathfrak{F}g)(\vec{a}',\vec{b}')\, \mathrm{d}^{2n}(\vec{a}',\vec{b}')\end{aligned}$$

Up to the exponential factor including $\hbar$, this is a convolution of thr functions $\mathfrak{F}f$ and $\mathfrak{F}g$. In the classical limit $\hbar \to 0$, the factor vanishes and $[\mathfrak{F}(f*g)](\vec{a},\vec{b}) = (2\pi)^{-n}[(\mathfrak{F}f)*(\mathfrak{F}g)](\vec{a}',\vec{b}')$, and by reversing the Fourier transform we find $f * g \overset{\hbar\to 0}{\to} fg$, i. e. the pointwise multiplication of the two functions. Note that the Moyal star product in non-commutative (as the multiplication of operators), but the multiplication of functions is.

3.5 Classical and quantum mechanics

We have seen some correspondence of classical and quantum mechanics and not want to check how well they fit together. To this aim, we shall formulate classical mechanics in a way which resembles quantum mechanics.

We consider a classical particle moving in space; we assume it to be point-like, i. e. it should not rotate in space etc. The movement of such particle is given its *trajectory* in configuration space $\vec{x} = \vec{x}(t) \in \mathbb{R}^3$.[5] The *velocity* is the

[5] This is the physicists notation that $\vec{x}$ is a function of time t, in mathematical terms $\vec{x} : \mathbb{R} \to \mathbb{R}^3$.

first, the *acceleration* the second derivative with respect to time t, i. e. $\vec{v} = \dot{\vec{x}}$ and $\vec{a} = \dot{\vec{v}} = \ddot{\vec{x}}$, respectively.

Newton's second law (colloquially, $F = ma$) is then written as $m\ddot{\vec{x}} = \vec{F}$, the *equation of motion*. This second-order differential equation is usually posed as an initial value-problem with two initial values $\vec{x}(0)$ and $\dot{\vec{x}}(0)$. Provided that the force $\vec{F}$ is is *conservative*, i. e. the integral over every closed path vanishes ($\oint \vec{F}(\vec{s})\,\mathrm{d}\vec{s} = 0$), we can write it as the negative gradient of a *potential* $V = V(\vec{r})$, i. e. $\vec{F} = -\mathrm{grad}\, V = -\nabla V$. In case the potential is time-independent, the *Hamiltonian function* is the total energy given by

$$H = T + V = \frac{\vec{p}^2}{2m} + V(\vec{r}), \tag{43}$$

where $T = \frac{1}{2}m\vec{v}^2 = \frac{\vec{p}^2}{2m}$ is the kinetic energy with $\vec{p} = m\vec{v}$ being the (kinematical) *momentum*. For the components of position there holds $\dot{x}_j = \frac{p_j}{m} = \frac{\partial}{\partial p_j}\frac{p_j^2}{2m}$, for those of the momentum $\dot{p}_k = m\dot{v}_k = m\ddot{x}_k = F_k = -\frac{\partial V}{\partial x_k}$. We have the Hamiltonian equations of motion[6]

$$\dot{x}_j = \frac{\partial H}{\partial p_j} \quad \text{and} \quad \dot{p}_k = -\frac{\partial H}{\partial x_k} \quad \text{with } j,\, k \in \{1, \ldots, n\}. \tag{44}$$

Using these first-order differential equations and initial values ($\vec{x}(0)$, $\vec{p}(0)$), we can completely describe the motion of the particle by a trajectory ($\vec{x}(t)$, $\vec{p}(t)$) in phase space $\mathbb{R}^3 \times \mathbb{R}^3$. Every measureable quantity of that particle must then be a function on that phase space, and a point ($\vec{x}$, $\vec{p}$) is a classical pure state on phase space (mixed states would then be probability distributions).

We shall rewrite this a bit; for this we use the Poisson brackets.

Definition 14 (Poisson brackets)**.**
Let f and g be real-valued C^∞-functions acting on $(\vec{x}, \vec{p}) \in \mathbb{R}^{2n}$. The Poisson bracket *is then defined as the real-valued C^∞-function*

$$\{f, g\} := \sum_{j=1}^{n} \left(\frac{\partial f}{\partial x_j} \cdot \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \cdot \frac{\partial g}{\partial x_j} \right).$$

Note that if the degree of f and g is n and m, the degree of the Poisson bracket is at most $n+m-2$. In particular, polynomials of degree at most 2 are closed with respect to the Poisson bracket (similar things hold for commutators), but those of degree 3 or larger do not.

[6] This is a somewhat clumsy way of derivation; the usual approach is using Lagrange functions of second kind for generalised coordinates and the Legendre transform.

The Poisson bracket is bilinear, skew-symmetric ($\{g,\, f\} = -\{f,\, g\}$) and fulfils the Jacobi identity $\{f,\, \{g,\, h\}\} + \{g,\, \{h,\, f\}\} + \{h,\, \{f,\, g\}\} = 0$, i. e. it has the structure of a Lie algebra. Morover, it fulfils the product rule of derivation $\{fg,\, h\} = f\,\{g,\, h\} + \{f,\, h\}\,g$. Since x_j and p_k can be viewed as functions on $(\vec{x},\, \vec{p})$ extracting the respective components, we find in particular $\{x_j,\, x_k\} = \{p_j,\, p_k\} = 0$ and $\{x_j,\, p_k\} = \delta_{jk}$.

Now if $(\vec{x},\, \vec{p})(t)$ is a trajectory in phase space fulfilling the Hamiltonian equations of motion and $f(\vec{x},\, \vec{p})$ a function, then

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial x_j} \frac{\mathrm{d}x_j}{\mathrm{d}t} + \frac{\partial f}{\partial p_j} \frac{\mathrm{d}p_j}{\mathrm{d}t} \right) = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial x_j} \frac{\partial H}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial H}{\partial x_j} \right) = \{f,\, H\} \quad (45)$$

In particular, setting $f = x_i$ or $f = p_j$, we get back the Hamiltonian equations of motion. Moreover,

$$\{x_i,\, g\} = \frac{\partial g}{\partial p_i} \quad \text{and} \quad \{p_i,\, g\} = -\frac{\partial g}{\partial x_i}. \quad (46)$$

The (Lie) algebraic rules for the Poisson brackets are essentially also fulfilled by the commutators on algebras.

3.6 Quantisation and Groenewold's theorem

We note that all these rules also hold true, if we replace the classical variables by their quantised operators and the Poisson brackets by commutators divided by $\mathrm{i}\hbar$. In particular, the Heisenberg equations of motion read

$$\mathrm{i}\hbar \frac{\mathrm{d}\hat{A}_H}{\mathrm{d}t} = [\hat{A}_H,\, \hat{H}] \quad (47)$$

and also the algebra of operators with the commutators forms a Lie algebra.

This motivates the substituion rule that $\{\,\cdot\,,\,\cdot\,\}$ is to be replaced by $[\,\cdot\,,\,\cdot\,]/\mathrm{i}\hbar$ while going from classical to quantum mechanics, though we have to remember that quantum mechanics is something new and cannot completely be described classically. We shall show that this rule cannot be true for all quantities.

The previous subsection has shown that the Weyl transformation has some properties which are desired. It remains to be checked that is is consistent with the substitution rule, i. e.

$$Q_W(\{f,\, g\}) = \frac{1}{\mathrm{i}\hbar}[Q_W(f),\, Q_W(g)] \quad (48)$$

i. e. it is a homomorphism of Lie algebras. It will be shown that this is not the case and, in fact, there is no such quantisation from $\mathbb{R}^{2n}$ to $\mathcal{B}(L^2(\mathbb{R}^n))$.

Theorem 15 (Groenewold's theorem)**.**
There is no linear mapping Q from polynomials to differential operators with constant coefficients on $\mathbb{R}^n$, such that $Q(1) = \mathbb{1}$, $Q(x_i) = \hat{x}_i$ and $Q(p_i) = \hat{p}_i$ hold for all $i \in \{1, \ldots, n\}$ and eq. (48) holds.

It will already fail on a polynomial of degree 4. We will only give s sketch of the proof. The proof will be done in three steps:

1. Equation (48) holds for the Weyl quantisation, if f and g are polynomials, and the degree of f is not larger than 2.

2. If Q fulfils the conditions of the theorem, $Q = Q_W$ on polynomials with degree not larger than 3.

3. We use the fact that $x^2p^2 = \frac{1}{9}\{x^3, p^3\} = \frac{1}{4}\{x^2p, xp^2\}$ and find a contradiction for $Q = Q_W$ by showing that $\frac{1}{9}[Q(x^3), Q(p^3)] \neq \frac{1}{4}[Q(x^2p), Q(xp^2)]$.

Step 1: For f of degree 0, f is constant, and both sides are zero. For degree 1, $f = x_i$ or $f = p_j$, and one can show (we do not)

$$Q_W(x_i g) = Q_W(x_i)Q_W(g) - \frac{\mathrm{i}\hbar}{2} Q_W\left(\frac{\partial g}{\partial p_i}\right) = Q_W(g)Q_W(x_i) + \frac{\mathrm{i}\hbar}{2} Q_W\left(\frac{\partial g}{\partial p_i}\right),$$

so that $[Q_W(x_i), Q_W(g)] = \mathrm{i}\hbar Q_W(\frac{\partial g}{\partial p_i}) = Q_W(\{x_i, g\})$. A similar result holds for $f = p_j$. For degree 2, we use homogeneous polynomials f_1 and f_2 of degree 1. It follows that

$$Q_W(f_1 f_2) = \frac{Q_W(f_1)Q_W(f_2) + Q_W(f_2)Q_W(f_1)}{2} \tag{49}$$

and

$$\begin{aligned}
[Q_W(f_1 f_2), Q_W(g)] &= \frac{1}{2}[Q_W(f_1)Q_W(f_2) + Q_W(f_2)Q_W(f_1),\, Q_W(g)] \\
&= \frac{1}{2}\Big(Q_W(f_1)[Q_W(f_2),\, Q_W(g)] + [Q_W(f_1),\, Q_W(g)]Q_W(f_2) \\
&\quad + Q_W(f_2)[Q_W(f_1),\, Q_W(g)] + [Q_W(f_2),\, Q_W(g)]Q_W(f_1)\Big),
\end{aligned}$$

so that we have reduced it to the degree-1 case. We now use in this case the property $Q_W(f_1)[Q_W(f_2), Q_W(g)] = Q_W(f_1)\frac{Q_W(\{f_2,g\})}{\mathrm{i}\hbar}$ etc. and the reverse of the derivation property to find $[Q_W(f_1 f_2), Q_W(g)] = \frac{Q_W(\{f_1 f_2, g\})}{\mathrm{i}\hbar}$, and by linearity this is all we need to show.

Step 2: From the initial conditions, we see that $Q = Q_W$ for degree-1 polynomials. For f of degree 2, set $Q(f) = Q_W(f) + q(f)$. Then, for g of degree 1, there holds

$$Q(\{f, g\}) = \frac{1}{\mathrm{i}\hbar}[Q(f), Q(g)] = \frac{1}{\mathrm{i}\hbar}[Q_W(f), Q_W(g)] + \frac{1}{\mathrm{i}\hbar}[q(f), Q_W(g)]. \quad (50)$$

The first term is $Q_W(\{f, g\})$ by assumption, and since the degree of $\{f, g\}$ is 1. Thus the second term is zero, and $q(f)$ commutes with all $\hat{x}_i$ and $\hat{p}_j$. Now we know that the associated exponential operators act irreducibly on $L^2(\mathbb{R}^n)$. In some analogy to Schur's lemma from representation theory, one can show that operators sommuting with all $\hat{x}_i$ and $\hat{p}_j$ must be multiples of unity, i. e. $q(f) = c_f \mathbb{1}$. Now, for f and g of degree 2. we find

$$Q(\{f, g\}) = [Q_W(f) + c_f \mathbb{1}, Q_W(g) + c_g \mathbb{1}] = Q_W(\{f, g\}) \quad (51)$$

Since every polynomial of degree 2 can be written as $\{f, g\}$ for two other degree-2 polynomials, $Q = Q_W$ for degree-2 polynomials.

Starting with degree-3 polynomials f and degree-1 g, the first argument similarly yields $Q(f) = Q_W(f) + c_f \mathbb{1}$ and for degree-2 g we then find again $c_f = 0$. The brackets $\{f, g\}$ with degrees 3 and 2 generate all polynomials of degree 3, so that $Q = Q_W$ for degree-3 polynomials.

Step 3: Contradiction: We consider the polynomial $f(\vec{x}, \vec{p}) = x_1^2 p_1^2 = \frac{1}{9}\{x_1^3, p_1^3\} = \frac{1}{3}\{x_1^2 p_1, x_1 p_1^2\}$ of degree 4 written in two ways as Poisson brackets. Since the polynomials in the Poisson brackets are of degree 3, we must have

$$\frac{1}{9}[Q_W(x_1^3), Q_W(p_1^3)] = \frac{1}{3}[Q_W(x_1^2 p_1), Q_W(x_1 p_1^2)]. \quad (52)$$

But this leads to a contradiction. For the left-hand side, we easily find $\frac{1}{9}(\hat{x}_1^3 \hat{p}_1^3 - \hat{p}_1^3 \hat{x}_1^3)$, and for the right-hand side we have to use the Weyl symmetrisation procedure. Since we want to find a contradiction, it suffices to apply these operators to some specific function. Taking a function f which is constant in some neighbourhood of zero, we can ignore all terms ending with a $\hat{p}$-operator due to the vanishing derivatives. The left hand side we find for the derivative in the neighbourhood of zero $-\frac{1}{9}(\frac{\hbar}{\mathrm{i}})^3 \frac{\mathrm{d}x_1^3}{\mathrm{d}x_1} = \frac{2}{3}\mathrm{i}\hbar^3$; similarly, we can do the calculation for the right-hand side and find $\frac{2}{3}\mathrm{i}\hbar^3 \neq \frac{1}{3}\mathrm{i}\hbar^3$.