Introduction to Quantum Mechanics

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Contents

Chapter 1

Classical mechanics

Here we summarise the necessary background from classical mechanics, and introduce some physical terminology that will repeatedly occur in the lecture.

1.1 Newton's second law

A classical particle has a *mass* m, and its *state* is described by its *position* $\vec{r} \in \mathbb{R}^3$ and its *velocity* $\vec{v} = \dot{\vec{r}} = \frac{\mathrm{d}\vec{r}}{\mathrm{d}t}$ or, often more conveniently, its *momentum* $\vec{p} = m\vec{v}$. *Newton's second law* connects the change of momentum to the external force $\vec{F}$:

$$\dot{\vec{p}} = m\ddot{\vec{r}} = \vec{F}. \tag{1.1}$$

This is a second order differential equation for the time-dependent position of a classical particle. The solution is uniquely determined by two initial conditions, for example the position and velocity at a given time. The solution $r(\vec{t})$ is called the *trajectory* of the particle.

It is often convenient to study a system's dynamics in the so-called *phase space*, the space of position and momentum coordinates. A *phase-space trajectory*, $(\vec{r}(t), \vec{p}(t))$ is a curve in phase space, that position and momentum coordinates trace as time evolves for a particular initial condition. A *phase (space) portrait* is a sketch of a collection of several phase-space trajectories belonging to different initial conditions, that summarise the overall types of trajectories.

1.2 Hamilton's canonical equations and phase space-dynamics

1.2.1 Hamilton's canonical equations

In many cases of interest the force can be expressed as the negative gradient of a scalar function $V(\vec{r})$, the *potential*, i.e.,

$$\vec{F}(\vec{r}) = -\vec{\nabla}V(\vec{r}). \tag{1.2}$$

Such systems are referred to as *conservative*, as they *conserve* the *energy*.

Remark 1. Remind yourself of the definitions and the physical units of *force*, *energy*, and *action*.

In what follows we shall for simplicity discuss one-dimensional systems, with coordinate $q \in \mathbb{R}$ and momentum $p \in \mathbb{R}$. For a conservative system Newton's second law (1.1) can then be written as

$$\dot{p} = -\frac{\partial V}{\partial q}, \tag{1.3}$$

and by definition we have

$$\dot{q} = \frac{p}{m}. \tag{1.4}$$

Introducing the function

$$H(p,q) = \frac{p^2}{2m} + V(q), \tag{1.5}$$

the dynamical equations (1.3) and (1.4) can be rewritten as

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \text{and} \quad \dot{q} = \frac{\partial H}{\partial p}. \tag{1.6}$$

These are *Hamilton's canonical equations*. The function $H(p,q)$ is called the *Hamiltonian* function, its value is the total energy of a system for a given state (p,q). The term $\frac{p^2}{2m}$ is the *kinetic energy*, $V(q)$ is the *potential energy*. Hamiltonian dynamics conserves the total energy, i.e., $\frac{\mathrm{d}H}{\mathrm{d}t} = 0$.

Remark 2. Hamiltonian mechanics applies more generally than in situations where $p = m\dot{q}$, i.e., q and p do not have to refer to physical coordinate and momentum in all situations (see *canonically conjugate variables* below). It does only apply in situations where the total energy is conserved. Thus, for example systems with friction or other losses *cannot* be described in the standard Hamiltonian formalism.

1.2.2 The potential and characteristics of the dynamics

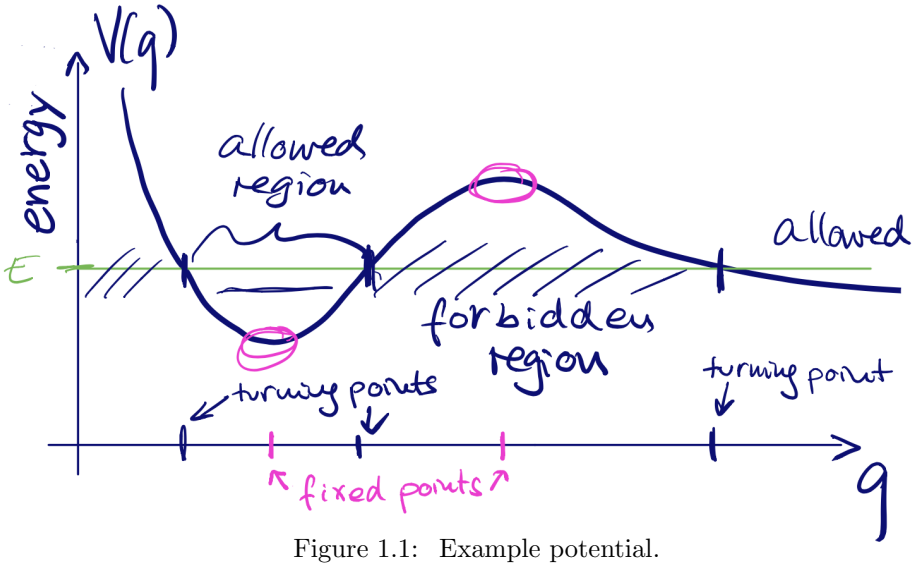
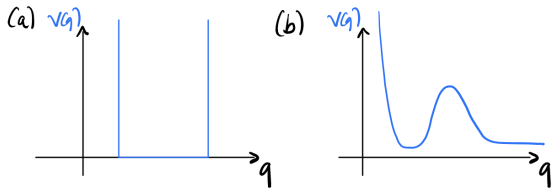


Figure 1.1: Example potential.

For systems whose Hamiltonian is of the form kinetic plus potential energy, as in equation (1.5), one can deduce basic properties of the dynamics from the potential, as sketched in figure 1.1. The extrema of the potential correspond to *fixed points* (or *equilibrium* configurations) of the dynamics. Minima are stable, and maxima are unstable fixed points. For a given energy a particle can only be in a region where its total energy is larger or equal to the potential energy. These regions are called *classically allowed*. They are separated by *turning points* from the *classically forbidden* regions, in which the potential is larger than the total energy available. In a classically allowed region that is bounded by two turning points, a particle oscillates between them. For a region that is only bound by one turning point, the particle comes in from one side, is reflected at the turning point and then moves away in the direction it came from, towards (negative or positive) infinity.

Exercise 1. Sketch the phase space portrait for a particle in one dimension with Hamiltonian of the form $\frac{p^2}{2m} + V(q)$ for the two potentials sketched here on the right.



Example 1 - The free particle. The free particle moves without an external potential, i.e., the Hamiltonian is given by $H = \frac{p^2}{2m}$. Thus, the canonical equations of motion become

$$\dot{p} = 0, \quad \text{and} \quad \dot{q} = \frac{p}{m}, \tag{1.7}$$

and we find $p = const$, and $q(t) = \frac{p}{m}t + q_0$. Sketch the phase space portrait!

Remark 3. $\dot{q} = \frac{p}{m}$ of course always holds for systems whose total energy is of the form $H = \frac{p^2}{2m} + V(q)$.

Remark 4. We could have also used the conservation of energy to deduce that the momentum is conserved here.

Example 2 - The harmonic oscillator. The harmonic oscillator is a particle in a quadratic potential, $V(q) \propto q^2$. It is a very important model system in physics for several reasons. Firstly, it has a simple analytical solution. Secondly, and more importantly, it is a good approximation for many systems that perform small oscillations around an equilibrium configuration. On a mathematical level this approximation can be interpreted as a Taylor expansion of the actual potential up to second order around a minimum, where the first derivative vanishes. The harmonic oscillator is for example a rough approximation for the vibrations of a two-atomic molecule.

Let us here consider the example of a mass m on a spring for small displacements from the equilibrium configuration. At equilibrium the spring counterbalances gravity and there is no net force acting on the mass. If the mass is displaced slightly, the spring responds with a compensation force which is proportional to the displacement (this is known as *Hooke's law*):

$$F = -Dq, \tag{1.8}$$

where D is the spring constant, and q denotes the displacement from equilibrium (i.e. q is positive when the spring is stretched). It is convenient to define a frequency $\omega = \sqrt{\frac{D}{m}}$. The potential is then given by

$$V(q) = \frac{D}{2}q^2 = \frac{m\omega^2}{2}q^2, \tag{1.9}$$

and we have the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2. \tag{1.10}$$

From the conservation of energy we can deduce the phase space portrait as consisting of concentric ellipses.

The equations of motion

$$\dot{p} = -m\omega^2 q, \quad \dot{q} = \frac{p}{m}, \tag{1.11}$$

can be combined into a single second-order differential equation for q,

$$\ddot{q} = -\omega^2 q. \tag{1.12}$$

With the initial conditions $q(t = 0) = q_0$ and $p(t = 0) = p_0$ the solution is given by

$$q(t) = q_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \tag{1.13}$$

$$p(t) = p_0 \cos(\omega t) - q_0 m\omega \sin(\omega t). \tag{1.14}$$

These equations describe *harmonic* oscillations.

1.3 Time evolution of general dynamical variables - Poisson brackets

The time evolution of any dynamical variable $A(p,q)$ is governed by the equation

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial q}\dot{q} + \frac{\partial A}{\partial p}\dot{p} + \frac{\partial A}{\partial t}. \tag{1.15}$$

Remark 5. For a quantity without explicit time dependence we have $\frac{\partial A}{\partial t} = 0$. All $A(p,q)$ are implicitly time dependent via the time dependence of p and q. Some variables, however, might in addition have an explicit time dependence. Take for example the potential energy in an oscillating potential of the form $V(q,t) = (q - \cos(\omega t))^2$.

Inserting Hamilton's canonical equations (1.6) into (1.15) we find

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial A}{\partial t} = \{H, A\} + \frac{\partial A}{\partial t}, \tag{1.16}$$

where we have defined the *Poisson bracket*, $\{\cdot,\cdot\}$ as

$$\{A, B\} = \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} - \frac{\partial A}{\partial q}\frac{\partial B}{\partial p}. \tag{1.17}$$

For N-dimensional systems the Poisson bracket is defined as

$$\{A, B\} = \sum_{j=1}^{N} \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j}. \tag{1.18}$$

Remark 6. Note that both this definition and the one where p and q are interchanged are used in the literature.

A dynamical variable without explicit time dependence is conserved in time if $\{H, A\} = 0$. Such quantities are also referred to as *constants of motion*. For the special case that H does not depend on one of the canonical variables q_j the corresponding p_j is conserved. Then q_j is called a *cyclic variable*.

1.3.1 Properties of Poisson brackets

The *Poisson bracket* has the following properties:

(i) $\{A, A\} = 0$ for all A

(ii) Linearity in the first element: $\{c_1 A + c_2 B, C\} = c_1\{A, C\} + c_2\{B, C\}$

(iii) Anti-symmetry with respect to interchange of elements: $\{A, B\} = -\{B, A\}$

(iv) Poisson-bracket with constant vanishes: $\{c, A\} = 0$, for c constant

(v) Leibniz rule (product rule): $\{AB, C\} = A\{B, C\} + \{A, C\}B$

(vi) Jacobi identity: $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$.

The Poisson bracket between momentum and position coordinates $\{p_j, q_k\} = \delta_{jk}$ is called the *fundamental* Poisson bracket. Every pair $P_j(p_l, q_m)$, $Q_j(p_l, q_m)$ that fulfils $\{P_j, Q_j\} = 1$ is a pair of *canonically conjugate variables* and one can use the Hamiltonian formalism where $H(P_j, Q_j)$ is the total energy of the system, even if this is different from $\frac{P^2}{2m} + V(Q)$. In general of course this also means that $\dot{Q} \neq \frac{P}{m}$.

Exercise 2. Verify that the Poisson bracket defined in (1.17) indeed fulfils all the above properties.

1.4 Historic excursion: The birth of quantum mechanics

In the late 19th century physics was regarded as "complete", in the sense that it was believed that Newton's laws, together with Maxwell's theory of electromagnetism explained *everything*, and all that was left was applying these theories to various situations. However, at the turn of the century some experiments were under way that revealed a fundamental lack of understanding. These included the measurement of atomic spectra, scattering experiments, the photo-electric effect, and the study of the light emitted from hot objects. These experiments and the attempts to build a corresponding theory led to the biggest revolution in modern physics, and the development of quantum mechanics.

Quantum theory is often divided into *old* and *modern* quantum theory. The name *old quantum theory* refers to the theory used in the initial 25 years of quantum theory, for example Bohr's theory of the atom, where electrons are confined to discrete orbits around the atomic nucleus, while there is no actual theoretical reason for this phenomenon given. While *old* quantum theory explained many of the experimental results, and introduced the concept of *energy quantisation*, there was no deeper understanding of the phenomena, and there were a number of unsolved paradoxes. In 1924/25 several breakthroughs were made, which led to the modern formulation of quantum theory (which, I want to mention such as not to mislead you, still has a lot of unresolved aspects, but we shall not focus on these.).

Werner Heisenberg (who was only 24 then) came up with a strange dynamical equation for observables (measurable quantities) that do not commute:

$$\dot{a} = \frac{2\pi \mathrm{i}}{h}(Wa - aW),$$

where a is an arbitrary observable (for example the position of a particle), and W denotes the energy. It later turned out that the idea of non-commutative objects is of course closely related to matrices, which were not very popular/well-known amongst physicists in the 1920's. Heisenberg's formulation of quantum mechanics is sometimes referred to as *matrix mechanics*.

In 1926 Schrödinger came up with his famous *wave equation*,

$$\mathrm{i}\frac{h}{2\pi}\dot{\psi}(\vec{r},t) = \left(-\frac{h^2}{8\pi^2 m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r},t),$$

where the complex function $\psi(\vec{r},t)$ is meant to somehow encode the position of a quantum particle, and the operator $-\frac{h^2}{2m}\nabla^2 + V(\vec{r})$ represents the energy. We shall discuss this further in section 2.

The fact that Schrödinger's and Heisenberg's theories are actually two different formulations of the same theory was not immediately clear. Around the same time as Schrödinger formulated his wave-theory, Dirac developed an abstract formulation of quantum theory, which unifies both Heisenberg and Schrödinger picture. All three of them received Nobel prizes for the development of quantum theory (Heisenberg in 1932, Dirac and Schrödinger jointly in 1933).

The development of the theory was very exciting for everyone involved. Legend has it that in the summer of 1925 Heisenberg was thinking hard about quantum mechanics but didn't make much progress. In addition he was suffering from bad hay fever, and decided to escape to Helgoland, an island in the northern sea. There he went for long hikes, read poetry, and also finally found his quantum theory! Later he wrote about this in his autobiography: *It was about 3 o'clock at night when the final result of the calculation lay before me. At first I was deeply shaken. I was so excited that I could not think of sleep. So I left the house and awaited the sunrise on the top of a rock.* He later sent his results to Wolfgang Pauli, with a letter saying: *Everything is still vague and unclear to me, but it seems as if the electrons will no longer move on orbits...*

Chapter 2

Schrödinger dynamics

In this chapter we provide a first introduction to Schrödinger's wave equation, the meaning and interpretation of the wave function etc. Much of the content will be formalised in chapter 4.

2.1 The Schrödinger equation and the wave function

In parallel to Heisenberg's formulation of quantum mechanics Schrödinger developed a description in terms of what is known as the *wave function*. He was inspired by Einstein's and de Broglie's ideas of *wave-particle-duality* and *matter waves*. In modern form this *time-dependent Schrödinger equation* is written as

$$\mathrm{i}\hbar\dot{\psi}(\vec{r},t) = \hat{H}\psi(\vec{r},t), \tag{2.1}$$

where the dot denotes the derivative with respect to time. Here $\hat{H}$ is the *Hamiltonian*, a differential operator acting on the *wave function* ψ, and $\hbar = \frac{h}{2\pi}$, where $h \approx 6.626 \times 10^{-34}$Js is Planck's constant. The Hamiltonian encodes the total energy of the system and is often of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}), \tag{2.2}$$

where ∇^2 denotes the Laplacian, i.e. in three dimensions in Cartesian coordinates, $\nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$. The first term encodes the kinetic and the second the potential energy. We will often consider one-dimensional systems for which the Schrödinger equation with a Hamiltonian of the form (2.2) takes the form

$$\mathrm{i}\hbar\dot{\psi}(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t). \tag{2.3}$$

Remark 7. In the context of quantum mechanics, we usually denote the spatial coordinate of one-dimensional systems, the argument of the wave function, by x.

2.1.1 The wave function

The wave function $\psi \in \mathbb{C}$ is interpreted as a *probability amplitude*. The square modulus of the wave function is a probability density. Specifically, $|\psi(x,t)|^2\mathrm{d}x$ is the probability of finding a quantum particle (described by the wave function ψ) between x and $x+\mathrm{d}x$ at time t (assuming ψ is *normalised* to one, that is, $\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x = 1$.). The normalisation condition $\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x = 1$ means that the particle is *somewhere* with probability one. The probability to find the particle in the interval $A = [a,b]$ is given by

$$\int_a^b |\psi(x)|^2\mathrm{d}x. \tag{2.4}$$

The wave function encodes everything that one can possibly know about a quantum particle. Knowing $\psi(x,t_0)$ one can deduce $\psi(x,t)$ for all times. That is, the time evolution in quantum mechanics is *deterministic*.

To interpret $|\psi(x,t)|^2$ as a probability distribution we need $\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x$ to be finite. That is, $\psi(x,t)\in L^2(\mathbb{R})$ (we refer to this as *normalisable* or *square integrable*).

Remark 8. We will mostly consider wave functions that are in L^2, but the theory can be slightly extended to include, for example, functions such as *plane waves*, $\psi\propto \mathrm{e}^{\mathrm{i}kx}$. We shall occasionally use such functions, and fill in a minimum of interpretational background when needed.

Remark 9. While it is meaningful to consider all square integrable functions as wave functions, as they lead to a probability density, there are other motivations that might restrict the space of admissible wave functions to certain subspaces of L^2. For example, the right-hand side of the Schrödinger equation (2.3) is only defined for functions $\psi(x)$ that are at least twice differentiable, which is not the case for all square integrable functions.

Exercise 3. Consider the wave function

$$\psi(x,t)=A\mathrm{e}^{-\lambda|x|}\mathrm{e}^{-\mathrm{i}\omega t},$$

where A,λ,ω are real positive constants.

(a) Find the value of A for which ψ is normalised to one.

(b) What is the probability to find the particle described by $\psi(x,t)$ in the interval $[-\frac{1}{\lambda},\frac{1}{\lambda}]$?

2.1.2 Probability current and conservation of probability

To interpret a time-dependent wave function that is a solution of the time-dependent Schrödinger equation as a probability amplitude, the overall norm should stay conserved over time. Let us now check whether this is indeed the case. We consider the total probability

$$\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x \tag{2.5}$$

as a function of time, assuming the Hamiltonian is of the form (2.2). In this context we can only consider wave functions that are at least twice differentiable. In this case, the derivative with respect to time and the integral over the coordinate x commute, that is, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x &= \int_{-\infty}^{\infty}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(x,t)|^2\mathrm{d}x\\ &= \int_{-\infty}^{\infty}\dot\psi^*(x,t)\psi(x,t)+\psi^*(x,t)\dot\psi(x,t)\mathrm{d}x,\end{aligned} \tag{2.6}$$

where the asterisk * denotes complex conjugation. Inserting the Schrödinger equation and its conjugate yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x &= \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}V(x)\psi^*(x,t)\psi(x,t)-\frac{\hbar^2}{2m}\psi''^*(x,t)\psi(x,t)\mathrm{d}x\\ &\quad -\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}V(x)\psi^*(x,t)\psi(x,t)-\frac{\hbar^2}{2m}\psi^*(x,t)\psi''(x,t)\mathrm{d}x\\ &= \frac{\mathrm{i}\hbar}{2m}\int_{-\infty}^{\infty}\psi^*(x,t)\psi''(x,t)-\psi''^*(x,t)\psi(x,t)\mathrm{d}x,\end{aligned} \tag{2.7}$$

where we have made use of the fact that the potential $V(x)$ is a real function. Now we recognise the integrand as the first derivative of a function which is proportional to the so-called *probability current* or *probability flux*, defined as

$$j(x,t):=\frac{\hbar}{2m\mathrm{i}}\left(\psi^*(x,t)\psi'(x,t)-\psi'^*(x,t)\psi(x,t)\right). \tag{2.8}$$

We can integrate to find

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x \quad = \quad -\big[j(x,t)\big]_{x=-\infty}^{x=\infty}. \tag{2.9}$$

That is, if $j(x)$ tends to zero for $x \to \pm\infty$ then the overall probability is indeed conserved in time. This condition is fulfilled as long as $\psi(x)$ tends to zero at infinity and its first derivative is bounded, in this case, the overall probability is conserved in time.

Remark 10. For those who are interested in the mathematical subtleties: we shall return to the discrepancy of the different spaces of admissible wave functions in later chapters. For those who do not wish to dwell too deeply into subtleties, it is of little (or no) harm to take the attitude of most physics textbooks, that any *physically meaningful* wave function is a square integrable function that also fulfils all the necessary conditions to make it normalisable, make sense of both sides of the Schrödinger equation, and conserve the norm over time.

2.1.3 Superposition principle

The Schrödinger equation is a linear differential equation. Thus, if $\psi_1(x,t)$ and $\psi_2(x,t)$ are solutions, and $c_1, c_2 \in \mathbb{C}$ are constants, then $c_1\psi_1(x,t) + c_2\psi_2(x,t)$ is also a solutions (Verify this!). This perhaps trivial sounding fact plays a central role in quantum theory. On a formal level it makes quantum mechanics much "easier" than classical mechanics.

2.1.4 The Hamiltonian and the energy

A quantum system is characterised by its *Hamiltonian* $\hat{H}$, an operator acting on the wave function, whose *expectation value*, defined as

$$\langle\hat{H}\rangle := \frac{\int_{-\infty}^{\infty}\psi^*(x,t)\hat{H}\psi(x,t)\mathrm{d}x}{\int_{-\infty}^{\infty}|\psi(x,t)|^2\mathrm{d}x}, \quad \text{(and analogously for higher dimensions)} \tag{2.10}$$

gives the *total energy* of the system.

For a Hamiltonian of the type (2.2), consisting of potential and kinetic energy, if the potential fulfills $V(x \to \pm\infty) \to \infty$, all eigenvalues (*eigenenergies*) of the Hamiltonian, are real numbers, and the corresponding eigenfunctions (also referred to as *eigenstates*) form an *orthonormal* basis for all possible wave functions of the system. The eigenstates $\phi_E(\vec{r})$ are the solutions of the *time-independent Schrödinger equation*

$$\hat{H}\phi_E(\vec{r}) = E\phi_E(\vec{r}). \tag{2.11}$$

Here *orthonormality* means that

$$\int_{\text{all space}}\phi_E^*(\vec{r})\phi_{E'}(\vec{r})\mathrm{d}V = \delta_{EE'}. \tag{2.12}$$

Remark 11. For potentials that are bounded (and don't go to infinity at infinity), the situation is more complicated. Here, typically the spectrum consists of discrete eigenvalues and a continuum part.

2.2 Stationary solutions: The time-independent Schrödinger equation

Consider special solutions of the time-dependent Schrödinger equation of the form

$$\psi(x,t) = \phi(x)\chi(t). \tag{2.13}$$

Inserting this ansatz into the Schrödinger equation yields

$$\mathrm{i}\hbar\frac{\dot{\chi}(t)}{\chi(t)} = \frac{\hat{H}\phi(x)}{\phi(x)}. \tag{2.14}$$

Since the left side of this equation is independent of x, so has to be the right side. Similarly, as the right side is independent of t, so is the left side, and in fact, both sides have to be constant. We call the constant E and separate the original equation into two differential equations

$$\mathrm{i}\hbar\dot{\chi}(t) = E\chi(t) \tag{2.15}$$
$$\hat{H}\phi(x) = E\phi(x). \tag{2.16}$$

Remark 12. This method is known as *separation of variables*.

Equation (2.15) is easily solved by direct integration to yield $\chi(t) = \chi(0)\mathrm{e}^{-\mathrm{i}Et/\hbar}$. Equation (2.16) is just the time-independent Schrödinger equation, that is, the eigenvalue equation for $\hat{H}$. The functions $\phi_E(x)$ are the eigenfunctions of $\hat{H}$ to the eigenvalues E. They are also referred to as *eigenstates*. We will solve some examples of this, especially in chapter 7. The eigenvalue equation can only be solved analytically for a small number of textbook cases.

Remark 13. For Hamiltonians of the form $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$, where the potential has the property $V(x \to \pm\infty) \to \infty$ normalisable solutions to the time-independent Schrödinger equation only exist for special discrete values of E. These discrete energies are the reason for the discrete atomic spectra, that is, the distinct colours that are emitted by stimulated atoms (think for example of fluorescent lamps).

The time-dependence of separable wave functions is rather trivial:

$$\psi(x,t) = \chi_0\mathrm{e}^{-\mathrm{i}Et/\hbar}\phi_E(x). \tag{2.17}$$

In particular, if the initial wave function at time zero is an eigenfunction of $\hat{H}$ we have $\chi_0 = 1$ and

$$\psi(x,t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\phi_E(x), \tag{2.18}$$

that is, an initial eigenstate evolves in time only by acquiring a phase factor, which means for the probability density

$$|\psi(x,t)|^2 = |\phi_E(x)|^2. \tag{2.19}$$

Hence, these wave functions are called *stationary states*.

Linear superpositions of stationary states, however, do have a non-trivial time-dependence. Consider for example an initial state which is a superposition of two eigenstates belonging to two different energies E_1 and E_2,

$$\psi(x,0) = a\phi_{E_1}(x) + b\phi_{E_2}(x).$$

The probability density of the time-dependent state is then given by

$$\begin{aligned}|\psi(x,t)|^2 =& |a|^2|\phi_{E_1}(x)|^2 + |b|^2|\phi_{E_2}(x)|^2 \\ &+ a^*b\,\mathrm{e}^{\mathrm{i}(E_1-E_2)t/\hbar}\phi^*_{E_1}(x)\phi_{E_2}(x) + ab^*\,\mathrm{e}^{\mathrm{i}(E_2-E_1)t/\hbar}\phi_{E_1}(x)\phi^*_{E_2}(x)\end{aligned} \tag{2.20}$$

The last two terms are time-dependent and are often referred to as the *interference terms*. In the special case where $a, b \in \mathbb{R}$, and also the eigenfunctions are real valued, $\phi_{E_j} \in \mathbb{R}$, this reduces to

$$|\psi(x,t)|^2 = a^2|\phi_{E_1}(x)|^2 + b^2|\phi_{E_2}(x)|^2 + 2ab\cos(\tfrac{E_2-E_1}{\hbar}t)\,\phi_{E_1}(x)\phi_{E_2}(x), \tag{2.21}$$

that is, the probability oscillates with a frequency determined by the energy difference of the two states in the superposition.

2.3 The method of stationary states

Consider an initial state that is an arbitrary superposition of eigenstates of the Hamiltonian

$$\psi(x, t = 0) = \sum_n a_n \phi_n(x), \tag{2.22}$$

with

$$\hat{H}\phi_n(x) = E_n \phi_n(x).$$

Due to the linearity of the Schrödinger equation, the time-dependent state is given by

$$\psi(x, t) = \sum_n a_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar} \phi_n(x). \tag{2.23}$$

Remark 14. That is the superposition principle again!

Given that the eigenstates of a Hamiltonian are a basis for all possible states of a system, and the superposition principle, the time-evolution of an arbitrary initial state can be deduced by representing it in the eigenbasis. This method is often called the *method of stationary states*.

2.3.1 The method of stationary states (for one dimensional systems in coordinate representation)

Given: Hamiltonian $\hat{H}$, initial wave function $\psi(x, t = 0)$
Wanted: Wave function at time t, $\psi(x, t)$

Method:

1. Calculate the eigenvalues E_n and normalised eigenstates $\phi_n(x)$ of the Hamiltonian $\hat{H}$.

2. Expand the initial wave function in the basis of eigenstates $\{\phi_n(x)\}$:

$$\psi(x, 0) = \sum_n a_n \phi_n(x).$$

   The coefficients are given by $a_n = \int_{-\infty}^{\infty} \phi_n^*(x)\psi(x, 0)dx$.

3. The time evolution is then given by

$$\psi(x, t) = \sum_n a_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar} \phi_n(x).$$

2.4 Example: Particle in a half box

(From David Tannor's Introduction to Quantum Mechanics)

A standard system in quantum mechanics is the so-called *particle in a box*. In one dimension that is a particle moving freely on a certain interval on the real line, here we consider the interval $[0, L]$. The Hamiltonian of the system is given by $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$, where there is an infinite potential outside this interval, i.e.

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty, & \text{otherwise.} \end{cases}$$

We shall discuss the solution of the time-independent Schrödinger equation for this system in chapter 7.3. For now we simply provide the result: The eigenvalues of the Hamiltonian are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \tag{2.24}$$

and the corresponding eigenfunctions are

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), & 0 \le x \le L \\ 0, \quad \text{otherwise.} \end{cases} \tag{2.25}$$

The first 5 eigenfunctions are schematically depicted at the height of their corresponding energies in figure 2.1.

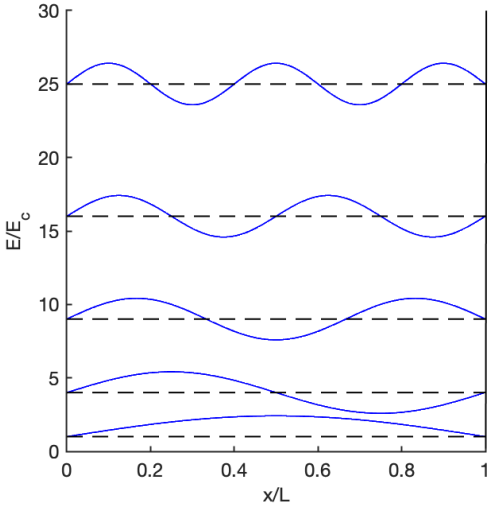


Figure 2.1: Eigenvalues and eigenfunctions of a particle in a box.

Remark 15. This is analogous to the problem of standing waves on a string.

Consider a quantum particle in the lowest eigenstate of a box potential of length L. Assume now that at time $t = 0$ the box is suddenly expanded to the length $2L$. If this is done infinitely fast, the wavefunction is initially not altered. However, the wavefunction is now not an eigenfunction of the new system, and thus it dynamically evolves for times $t > 0$.

Remark 16. Such a fast change of the external potential in an experiment is often called a *quantum quench*, a method often employed to experimentally prepare a system in a state other than an eigenstate.

We can use the method of stationary states to understand the dynamics of the wave function. It turns out that the motion of the wave function while being rather complicated in its details, is periodic. Let us use the method of stationary states to calculate the shortest time τ at which $\psi(x,\tau) = \psi(x,0)$. For this purpose we need to expand the wave function at time zero, which is a normalised eigenfunction of the square well of length L,

$$\psi(x,0) = \phi_1^{(L)}(x), \tag{2.26}$$

in the basis of eigenfunctions $\phi_n^{(2L)}(x)$ of the square well of twice the size, that is, we write

$$\phi_1^{(L)}(x) = \sum_n a_n \phi_n^{(2L)}(x). \tag{2.27}$$

To calculate the actual coefficients a_n we would have to calculate the integrals

$$a_n = \int_{-\infty}^{\infty} \phi_n^{*(2L)}(x)\phi_1^{(L)}(x)\mathrm{d}x = \frac{\sqrt{2}}{L}\int_0^L \sin\left(\frac{n\pi x}{2L}\right)\sin\left(\frac{\pi x}{L}\right)\mathrm{d}x. \tag{2.28}$$

However, to calculate τ we do not need to know all the values of a_n. The wave function at time t has the form

$$\psi(x,t) = \sum_n a_n \mathrm{e}^{-\mathrm{i}E_n^{(2L)}t/\hbar}\phi_n^{(2L)}(x). \tag{2.29}$$

Inserting the energy values for the square well of width $2L$, we have

$$\psi(x,t) = \sum_n a_n \mathrm{e}^{-\mathrm{i}\frac{\pi^2\hbar}{8mL^2}n^2 t}\phi_n^{(2L)}(x). \tag{2.30}$$

Or

$$\psi(x,t) = \sum_n a_n \mathrm{e}^{-\mathrm{i}\omega n^2 t}\phi_n^{(2L)}(x), \tag{2.31}$$

where we have defined $\omega = \frac{\pi^2\hbar}{8mL^2}$. Thus, we have $\psi(x,\tau) = \psi(x,0)$ at times τ for which all $\mathrm{e}^{-\mathrm{i}\omega n^2\tau} = 1$, which is true if all $n^2\omega\tau$ are integer multiples of 2π. Since n are integers here, the shortest such time τ thus fulfils

$$\tau = \frac{2\pi}{\omega} = \frac{16mL^2}{\hbar\pi}. \tag{2.32}$$

Chapter 3

Excursion: Mathematical background

After having gained some first impressions of quantum behaviour looking at Schrödinger's wave functions, we shall now move to a more abstract and versatile formulation of quantum mechanics, that will allow us to identify which questions can be answered by quantum mechanics, and which questions the theory does not "allow" us to ask. In particular in chapter 4 we will learn five principles/postulates of quantum mechanics that form the basis of the whole theory and its interpretations. Several mathematical concepts and notations are needed to formulate and understand these principles, and in the present chapter we provide the minimum background. Let us first, however, have a brief look into the first two postulates that we will discuss in more detail in chapter 4 to get an idea which mathematical background is needed and why.

3.1 States and obervables - Hilbert spaces and Hermitian operators

The main ingredients for this theoretical framework of quantum mechanics are the concepts of a state and of observables. A *state* encodes all the information one can have about a quantum system. *Observables* are measurable quantities (such as, for example, the position of a particle or its kinetic energy). In some ways, the same concepts appear in classical mechanics, but we so naturally associate the mathematical objects that describe these properties with the actual physical properties that they are seldom talked about.

Looking back at Hamilton's classical mechanics we see that all measurable quantities, i.e. *observables* are given by real phase-space functions, that is, real functions of the canonical variables. The canonical variables, in turn, are the classical *state*. We implicitly consider this state to be a property of the system (for example a particle) in classical physics, and talk about the *position of an object* or the *momentum of a particle*, in similar terms as when considering its mass, colour or other inherent property. In quantum mechanics we will have to let go of this.

The state of a quantum system, as defined above, encodes all we can in principle measure about a particle, but it makes no claim about measurable quantities being *properties of* a particle. We have already encountered this in the last chapter where we have seen that it makes little sense in Schrödinger's framework of quantum mechanics to talk about a *particle's position*. The only thing we can talk about is the *probability of finding a particle in a certain region at a given time.* Think this over - it is the essence of quantum mechanics!

As Philip Ball argues in his beautiful recent book "Beyond weird", this is neither weird nor strange. It does, however, require a shift away from century-old ways of thinking about the nature of things. This allows us to predict a lot of experimental observations with unprecedented accuracy, and to design technological devices such as transistors and lasers, that would be impossible on the basis of classical physics. A lot can be said (and over the decades a lot has been said, indeed) about the philosophical aspects of quantum theory. Here, however is not the place to do so. Let us instead focus on the mathematical framework and on what we *can* calculate with it.

As we shall see, compared to classical mechanics, the role of position and momentum is shifted from the state to observables. The role of the state is taken over by another mathematical object that does not appear explicitly in classical physics. That brings us to

The first principle of quantum mechanics: The state of a quantum system is described by a non-zero vector in a Hilbert space.

Observables are covered by

The second principle of quantum mechanics: A measurable quantity is described by a Hermitian operator on the Hilbert space. Both the measurable quantities and the operators representing them are often referred to as *observables*.

With this in mind in this chapter we shall review some general concepts from linear algebra and analysis, and in particular provide a minimal background on Hilbert spaces and Hermitian operators. We shall also learn about a very powerful notation for vectors and operators on Hilbert spaces that has been developed by Dirac especially for quantum mechanics, aptly called the *Dirac notation*, that we shall make use of in the rest of the course.

3.2 Some linear algebra and analysis

Here we summarise a few definitions from linear algebra that are essential in the abstract formulation of quantum mechanics.

Complex vector space: A set of elements (*vectors*) V, forming an Abelian (i.e. commutative) group with respect to addition $u+v$, and a scalar multiplication $\mathbb{C}\times V\to V$, satisfying

$$\begin{aligned}(\lambda+\mu)v &= \lambda v+\mu v\\ (\lambda\mu)v &= \lambda(\mu v)\\ \lambda(u+v) &= \lambda u+\lambda v\\ 1v &= v.\end{aligned}$$

for all $\lambda,\mu\in\mathbb{C}$ and $u,v\in V$, is called a vector space.

Remark 17. In general a vector space can be defined over any field $\mathbb{F}$, where the scalars are elements of $\mathbb{F}$. Most commonly encountered in physics are vector spaces over the real or the complex numbers.

Inner product space: An inner product space is a vector space V together with a map $V\times V\to\mathbb{C}$, written as (u,v), such that for all $u,v,w\in V$ and $\lambda,\mu\in\mathbb{C}$:

$$\begin{aligned}(u,v) &= (v,u)^*\\ (u,u) &\geq 0,\quad \text{and}\quad (u,u)=0\Leftrightarrow u=0\\ (u,\lambda v+\mu w) &= \lambda(u,v)+\mu(u,w).\end{aligned}$$

Linear (in)dependence, basis, dimension: A set of vectors $\{u_n\}$ is said to be *linearly independent* if no nontrivial linear combination of them sums to zero. If the set is on the contrary *linearly dependent*, one can express one member of the set as a linear combination of the others: $u_k=\sum_{n\neq k}\alpha_n u_n$.

The maximum number of linearly independent vectors in a space is called the *dimension* of the space.

A maximal set of linearly independent vectors is called a *basis*. That is, every vector in the space can be represented as a linear combination of the basis vectors: $\phi=\sum_n\phi_n u_n$. The ϕ_n are the *coefficients* or *components* of ϕ in the basis $\{u_n\}$. One can represent ϕ as an N-tuple of complex numbers, $(\phi_1,\dots,\phi_N)\in\mathbb{C}^N$, where N is the dimension of the vector space.

Norm: The norm $||v||$ of a vector can be defined via $||v||^2 = (v, v)$. A vector is called *normalised* if $||v|| = 1$.

Orthonormality: Two vectors u, v are called *orthogonal* if $(u, v) = 0$. A set of vectors $\{u_n\}$ is said to be *orthonormal* if each vector is normalised and the vectors are pairwise orthogonal.

An orthonormal maximal set of linearly independent vectors is an *orthonormal basis*.

Coefficients: The coefficients of a vector ϕ in an orthonormal basis $\{u_n\}$ can be found via the orthonormality condition as $\phi_n = (u_n, \phi)$.

Hilbert space: A Hilbert space $\mathcal{H}$ is a complex inner product space which is complete with respect to the norm induced by the inner product.

Completeness of a vector space: A vector space V is complete if the following holds. Whenever $\{u_n \in V\}$ is a sequence of vectors such that for any positive ϵ there exists an integer N_ϵ with

$$||u_m - u_n|| < \epsilon, \quad \text{for all } m, n > N_\epsilon,$$

then there exists a limit vector $u \in V$, such that

$$||u_n - u|| \to 0.$$

A finite dimensional vector space is automatically complete, i.e. every finite dimensional vector space is a Hilbert space.

Separable Hilbert space: A Hilbert space is called *separable* if it possesses a countable basis. In quantum mechanics, we deal only with separable Hilbert spaces.

Linear Operator: An operator on a vector space is a map $V \to V$. A *linear operator* A satisfies

$$A(\lambda u + \mu v) = \lambda(Au) + \mu(Av),$$

for all $\lambda, \mu \in \mathbb{C}$, and $u, v \in V$.

A linear operator on a finite dimensional vector space can be represented by a matrix.

Bounded operators An operator A on a Hilbert space is *bounded* if and only if there exists a real number $c > 0$, such that for all $u \in \mathcal{H}$,

$$||Au|| \leq c||u||.$$

Domain The domain $\mathcal{D}(A) \in \mathcal{H}$ of an operator A is the set of vectors on which A is bounded, i.e., the set of vectors $u \in \mathcal{H}$ for which $Au \in \mathcal{H}$.

Adjoint Operator: The *adjoint* $A^\dagger$ of a linear operator A is defined by the relation

$$(A^\dagger u, v) = (u, Av), \quad \text{for all } v \in \mathcal{D}(A) \text{ and } u \in \mathcal{D}(A^\dagger).$$

The adjoint fulfils the following properties:

$$(cA)^\dagger = c^* A^\dagger$$
$$(A + B)^\dagger = A^\dagger + B^\dagger$$
$$(AB)^\dagger = B^\dagger A^\dagger.$$

Hermiticity and Self-adjointness: A linear operator defined on a Hilbert space $\mathcal{H}$ is called *Hermitian*

$$(Au, v) = (u, Av), \quad \text{for all } v, u \in \mathcal{D}(A),$$

that is if $A^\dagger = A$ on the overlap of the domains of A and $A^\dagger$.

For bounded operators the domain is the whole Hilbert space, and Hermiticity leads to many useful properties. For unbounded operators, on the other hand, Hermiticity is not enough to guarantee some crucial properties we need in quantum mechanics. Here the stronger concept of *self-adjointness* is important. An operator A is *self-adjoint* if $A = A^\dagger$ and $\mathcal{D}(A) = \mathcal{D}(A^\dagger)$.

For more details, see, e.g. Ballentine, Cohen Tannoudji, or Brian Hall's "Quantum mechanics for Mathematicians".

Eigenvalues and eigenvectors: If an operator acting on a certain vector produces a scalar multiple of that same vector,

$$Au = au,$$

we call the vector u an *eigenvector* and the scalar a an *eigenvalue* of the operator A.

If A is an $N \times N$ matrix the eigenvalue equation only has nontrivial solutions if

$$\det(A - a\mathbb{1}) = 0.$$

This yields the *characteristic polynomial of* A, which is a polynomial of Nth order in a.

3.3 The Dirac notation

3.3.1 The dual space and the Riesz theorem

To any linear vector space V there exists a *dual space* of *linear functionals* on V. A linear functional F assigns a scalar $F(\phi)$ to each vector ϕ, such that

$$F(\alpha\phi + \beta\psi) = \alpha F(\phi) + \beta F(\psi), \tag{3.1}$$

for $\alpha, \beta \in \mathbb{C}$ and $\phi, \psi \in V$.

The set of linear functionals is itself a linear vector space V' with the definition

$$(F_1 + F_2)(\phi) = F_1(\phi) + F_2(\phi). \tag{3.2}$$

Theorem 1 (Riesz representation theorem)**.** *A complex Hilbert space $\mathcal{H}$ is anti-isomorphic to its dual space $\mathcal{H}'$. That is, there exists a one-to-one correspondence between linear functionals F and vectors f, such that all linear functionals can be represented in the form $F(\phi) = (f, \phi)$ with a fixed vector f and arbitrary vectors ϕ.*

We shall prove the Riesz theorem for separable Hilbert spaces here, making use of the fact that they possess a countable orthonormal basis. Clearly every vector defines a functional via the inner product. The proof for the opposite direction, that every functional can be represented as an inner product with a fixed vector, works by construction:

Proof. Let $\{\phi_n\}$ be an orthonormal basis of $\mathcal{H}$. Let $\psi = \sum_n \psi_n \phi_n$ with $\psi_n \in \mathbb{C}$ be an arbitrary vector in $\mathcal{H}$. Then

$$F(\psi) = \sum_n \psi_n F(\phi_n). \tag{3.3}$$

Defining the vector $f = \sum_n [F(\phi_n)]^* \phi_n$ we see that

$$(f, \psi) = \sum_n F(\phi_n)\psi_n = F(\psi) \tag{3.4}$$

for all $\psi \in \mathcal{H}$. □

3.3.2 The Dirac notation

Vectors in $\mathcal{H}$ are called *ket* vectors, written as $|\phi\rangle$, vectors in the dual space $\mathcal{H}'$ (functionals) are called *bra* vectors, written as $\langle f|$. In this way we have

$$F(\phi) = (f, \phi) = \langle f|\phi\rangle, \tag{3.5}$$

where the last expression is a "bra-ket" – hence the name.

Remark 18. On some level one can think of this *Dirac notation* simply as a notation for scalar products, but it turns out to be useful far beyond this.

There is an *anti-linear correspondence* between bras and kets due to the nature of the scalar product:

$$\alpha^*\langle f_1| + \beta^*\langle f_2| \longleftrightarrow \alpha|f_1\rangle + \beta|f_2\rangle. \tag{3.6}$$

Recalling the definition of the adjoint operator $\hat{A}^\dagger$ of a linear operator $\hat{A}$ we see that the bra associated to the ket vector $\hat{A}|\phi\rangle$ is the vector $\langle\phi|\hat{A}^\dagger$. That is, we can interpret the expression $\hat{A}|\phi\rangle$ as "$|\hat{A}\phi\rangle$" and the expression $\langle\phi|\hat{A}^\dagger$ as "$\langle\hat{A}\phi|$". That is, the notation $\langle\phi|\hat{A}|\psi\rangle$ denotes two equal, but morally different, things:

(i) The inner product of the vector ϕ with the vector resulting from acting with $\hat{A}$ on the vector ψ, i.e. "$\langle\phi|\hat{A}\psi\rangle$";

(ii) The inner product of the vector resulting from acting with $\hat{A}^\dagger$ onto the vector ϕ with the vector ψ, i.e. "$\langle\hat{A}^\dagger\phi|\psi\rangle$".

The definition of the adjoint operator is expressed in Dirac notation as

$$\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\phi\rangle^*. \tag{3.7}$$

3.3.3 Rules for finding the adjoint of an expression

To find the *adjoint* of an expression, one needs to

- complex conjugate scalars $c \leftrightarrow c^*$,
- replace kets with bras and vice versa $|\phi\rangle \leftrightarrow \langle\phi|$,
- replace operators with their adjoints $\hat{A} \leftrightarrow \hat{A}^\dagger$,
- reverse the order of factors.

As an example, consider the expression

$$c|\psi\rangle\langle\phi|A|\psi\rangle\langle\phi|.$$

This expression is an operator. The adjoint operator is given by

$$c^*|\phi\rangle\langle\psi|\hat{A}^\dagger|\phi\rangle\langle\psi|. \tag{3.8}$$

3.3.4 The outer product of two vectors

Besides the *inner product* of a bra $\langle\phi|$ and a ket $|\psi\rangle$, $\langle\phi|\psi\rangle$, which is a scalar, there is also an *outer product*, $|\psi\rangle\langle\phi|$, which is a linear operator.

Exercise 4. What is the adjoint operator of $|\psi\rangle\langle\phi|$?

Remark 19. An operator of the form $P = |\phi\rangle\langle\phi|$ is a *projection* operator, as the mapping $P : |\psi\rangle \mapsto \langle\phi|\psi\rangle|\phi\rangle$ is the projection of $|\psi\rangle$ onto $|\phi\rangle$. We will return to a more general notion of projection operators in the discussion of principle 4 in chapter 4.

3.3.5 Completeness and resolution of identity

An orthonormal set of vectors $\{\phi_n\}$ is complete if an arbitrary $|v\rangle \in V$ can be written as

$$|v\rangle = \sum_n v_n |\phi_n\rangle. \tag{3.9}$$

The coefficients v_n are given by

$$v_n = \langle\phi_n|v\rangle. \tag{3.10}$$

Reinserting this into the expansion (3.9) of $|v\rangle$ gives the identity

$$|v\rangle = \sum_n |\phi_n\rangle\langle\phi_n|v\rangle. \tag{3.11}$$

This, however, is identical to the statement

$$|v\rangle = \left(\sum_n |\phi_n\rangle\langle\phi_n|\right)|v\rangle. \tag{3.12}$$

Since this is valid for all vectors $v \in V$, that means that

$$\sum_n |\phi_n\rangle\langle\phi_n| = \mathbb{1}. \tag{3.13}$$

This property which is fulfilled by any complete orthonormal set, is called the *resolution of identity*.

3.4 More on Hermitian operators

Theorem 2. *All eigenvalues of a Hermitian operator are real.*

Proof. Consider the (non-zero) eigenvector $|u\rangle$ of a Hermitian operator $\hat{A} = \hat{A}^\dagger$, corresponding to the eigenvalue $a \neq 0$:

$$\hat{A}|u\rangle = a|u\rangle.$$

The adjoint equation reads

$$\langle u|\hat{A} = \langle u|a^*.$$

We have

$$\langle u|\hat{A}|u\rangle = \langle u|a|u\rangle = a\langle u|u\rangle.$$

On the other hand we have $\hat{A} = \hat{A}^\dagger$, and thus

$$\langle u|\hat{A}|u\rangle = \langle u|\hat{A}^\dagger|u\rangle = \langle u|a^*|u\rangle = a^*\langle u|u\rangle.$$

It follows that

$$a\langle u|u\rangle = a^*\langle u|u\rangle. \tag{3.14}$$

Since $\langle u|u\rangle \neq 0$ it follows that

$$a = a^* \in \mathbb{R}.$$

□

Theorem 3. *Eigenvectors of a Hermitian operator belonging to different eigenvalues are orthogonal.*

Exercise 5. Prove theorem 3.

Theorem 4. *The expectation values, $\langle v|\hat{A}|v\rangle$, of Hermitian operators are real. On the other hand, if every expectation value of an operator is real, the operator is Hermitian.*

We will prove theorem 4 in the lecture.

Finally, without proof, we state the following important

Theorem 5. *The eigenvectors of a Hermitian operator form a complete orthogonal basis set for the Hilbert space the operator acts upon.*

An operator A is called *anti-Hermitian* if $\hat{A}^\dagger = -\hat{A}$. If $\hat{A}$ is Hermitian then $\mathrm{i}\hat{A}$ is anti-Hermitian. Every operator can be uniquely decomposed into a Hermitian and an anti-Hermitian part, $\hat{A} = \hat{A}_h + \mathrm{i}\hat{A}_a$, with $\hat{A}_h^\dagger = \hat{A}_h$ and $\hat{A}_a^\dagger = \hat{A}_a$.

3.5 Vector/matrix representation

Consider a Hilbert space $\mathcal{H}$ with a countable orthonormal basis $\{|u_n\rangle\}$. The ket vectors $|\psi\rangle \in \mathcal{H}$ can be represented by (possibly infinite) column vectors of their coefficients in this basis:

$$|\psi\rangle = \sum_n a_n |u_n\rangle, \quad |\psi\rangle \simeq \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_j \\ \vdots \end{pmatrix} =: \vec{a}.$$

For the scalar product of two vectors $|\psi\rangle = \sum_n a_n|u_n\rangle$, and $|\phi\rangle = \sum_n b_n|u_n\rangle$ it follows from $\langle\phi| = \sum_n \langle u_n|b_n^*$ that

$$\begin{aligned} \langle\phi|\psi\rangle &= \sum_{m,n} \langle u_m|b_m^* a_n|u_n\rangle = \sum_{m,n} b_m^* a_n \langle u_m|u_n\rangle \\ &= \sum_{m,n} b_m^* a_n \delta_{mn} = \sum_n b_n^* a_n \\ &= (\vec{b}^*)^T \vec{a}\,. \end{aligned}$$

Similarly linear operators on the Hilbert space can be represented by matrices. Consider, e.g., the equation $\hat{M}|\psi\rangle = |\phi\rangle$, that is

$$\sum_n a_n \hat{M}|u_n\rangle = \sum_n b_n |u_n\rangle.$$

Operating on this with $\langle u_m|$ yields

$$\begin{aligned} \sum_n a_n \langle u_m|\hat{M}|u_n\rangle &= \sum_n b_n \langle u_m|u_n\rangle \\ \sum_n a_n \langle u_m|\hat{M}|u_n\rangle &= \sum_n b_n \delta_{mn} \\ \sum_n M_{mn} a_n &= b_m, \end{aligned}$$

which is valid for all m. Thus,

$$\hat{M}|\psi\rangle = |\phi\rangle \;\Leftrightarrow\; M\vec{a} = \vec{b},$$

with $\hat{M} = (M_{mn})$ and $M_{mn} = \langle u_m|\hat{M}|u_n\rangle$. In matrix representation Hermiticity means that $M_{mn} = M_{nm}^*$.

Chapter 4

The Principles of Quantum Mechanics

In this chapter we will learn about the five principles/postulates of quantum mechanics that allow an abstract formulation of the theory. The first two principles that we have already briefly encountered in the previous chapter, concern the description of the *states* of a quantum system and its *observables*, that is, its measurable quantities. The third and fourth principle concern the concept of *measurements* and the final one the *time-evolution* of quantum systems.

4.1 States and observables

A *state* encodes all the information one can have about a quantum system. *Observables* are measurable quantities (such as, for example, the position of a particle or its kinetic energy).

4.1.1 Principle 1 (States):

The state of a quantum system is described by a non-zero vector in a Hilbert space.

Remark 20. The space of square-integrable functions L^2 that we have dealt with in Schrödinger's theory of wave functions is a Hilbert space.

The superposition principle means that the sum of two states is a state, which also follows from the vector space properties. Two vectors describe the same state if they are complex multiples of each other. The equivalence class $\psi \to c\psi$ with $c \in \mathbb{C}$ defines *rays* through the "origin" of the Hilbert space. The space of these rays is called the *projective Hilbert space*.

Remark 21. Some caution is needed when dealing with the concept of the projective Hilbert space; while the states $\mathrm{e}^{\mathrm{i}\phi_1}\psi_1$ and $\mathrm{e}^{\mathrm{i}\phi_2}\psi_2$ are equivalent to the states ψ_1 and ψ_2 respectively, in general $\mathrm{e}^{\mathrm{i}\phi_1}\psi_1 + \mathrm{e}^{\mathrm{i}\phi_2}\psi_2$ describes a different state from $\psi_1 + \psi_2$.

4.1.2 Principle 2 (Observables):

A measurable quantity is described by a Hermitian operator on the Hilbert space. Both the measurable quantities and the operators representing them are often referred to as *observables*.

In particular the operators corresponding to *position* and *momentum*, $\hat{q}$ and $\hat{p}$, fulfil the commutation relation

$$[\hat{q}, \hat{p}] = \mathrm{i}\hbar\mathbb{1}, \tag{4.1}$$

where the *commutator* $[\cdot, \cdot]$ is defined as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}, \tag{4.2}$$

and $\mathbb{1}$ denotes the identity operator.

4.2 Measurement and dynamics

The first two principles state that a quantum state is a vector and that measurable quantities are represented by operators. Now we will focus on the actual measurement and how the outcome of a measurement is related to the operator describing an observable and the state describing the system.

4.2.1 Principle 3 ("Born rule"):

The possible outcomes of a measurement of an observable A are given by the eigenvalues of the corresponding operator $\hat{A}$. The probability of obtaining an eigenvalue a_j as a measurement outcome is encoded in the state $|\psi\rangle$ the system is in immediately before the measurement. The probability is given by $p(a_j) = \langle\psi|\hat{P}_j|\psi\rangle$, where $\hat{P}_j$ is the *projection operator* onto the subspace associated to the eigenvalue a_j. For non-degenerate, discrete eigenvalues this reduces to the modulus square $|\psi_j|^2$ of the coefficient of the (normalised) wave function $|\psi\rangle$ in the basis of eigenstates $|\phi_j\rangle$ of $\hat{A}$:

$$|\psi\rangle = \sum_n \psi_n|\phi_n\rangle, \quad \text{with} \quad \hat{A}|\phi_n\rangle = a_n|\phi_n\rangle. \tag{4.3}$$

For continuous spectra we replace the sum with an integral: The probability to obtain a value in the interval I in a measurement is the integral over the modulus squared of the components of the wave function over this interval $P = \int_I |\psi(\alpha)|^2 \mathrm{d}\alpha$, where

$$|\psi\rangle = \int \mathrm{d}\alpha\, \psi(\alpha)|\phi(\alpha)\rangle, \quad \text{with} \quad \hat{A}|\phi(\alpha)\rangle = \alpha|\phi(\alpha)\rangle. \tag{4.4}$$

4.2.2 Projection operator

A linear operator $\hat{P}$ that satisfies $\hat{P}^2 = \hat{P}$ is called a *projection operator*. Examples are operators of the form $\hat{P} = \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n|$ where $\{|\phi_n\rangle\}$ is an orthonormal set of vectors. We can easily verify that indeed $\hat{P}^2 = \hat{P}$:

$$\begin{aligned} \hat{P}^2 &= \sum_n |\phi_n\rangle\langle\phi_n| \sum_m |\phi_m\rangle\langle\phi_m| = \sum_{n,m} |\phi_n\rangle\langle\phi_n|\phi_m\rangle\langle\phi_m| \\ &= \sum_{n,m} \delta_{mn}|\phi_n\rangle\langle\phi_n| = \sum_n |\phi_n\rangle\langle\phi_n| = \hat{P} \qquad \square \end{aligned} \tag{4.5}$$

Exercise 6. Verify that the eigenvalues λ of a projection operator are either one or zero.

Example - Energies of a particle in a box of length L

The eigenvalues of the Hamiltonian are given by $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$. If the state is given by $|\psi\rangle = \sum_n \psi_n|\phi_n\rangle$ with $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$ we will obtain the value E_n in an energy measurement with probability $|\psi_n|^2$. If the system is in the "ground state" (that is, the state with the lowest energy, in this case E_1), for example, we will obtain the value $E_1 = \frac{\pi^2\hbar^2}{2mL^2}$ with probability one.

Expectation values

The *mean value* of the outcome of many measurements of an observable A on *identically prepared systems* does not have to be an eigenvalue of the operator $\hat{A}$. It is given by the *expectation value* of $\hat{A}$ in the state $|\psi\rangle$:

$$\langle\hat{A}\rangle := \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{4.6}$$

Let us verify this for the case of discrete eigenvalues: Let us denote the eigenvalues of $\hat{A}$ by a_n and the corresponding eigenvectors by $|\phi_n\rangle$, that is, $\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle$. The eigenvectors belonging

to different eigenvalues are automatically orthogonal, in addition we can choose them normalised. The mean value of many measurements is clearly given by

$$\langle \hat{A} \rangle = \sum_j a_j P(a_j), \tag{4.7}$$

where $P(a_j)$ denotes the probability that a measurement yields the outcome a_j. Let us now verify that this is indeed equal to the expression (4.6), using that according to principle 3 $P(a_j)$ is given by

$$\begin{aligned} P(a_j) &= |\langle \phi_j | \psi \rangle|^2 \\ &= \langle \psi | \phi_j \rangle \langle \phi_j | \psi \rangle, \end{aligned} \tag{4.8}$$

if the system is in the normalised state $|\psi\rangle$. Inserting expression (4.8) for the probability of the measurement outcome a_j into equation (4.7) yields

$$\begin{aligned} \langle \hat{A} \rangle &= \sum_j a_j \langle \psi | \phi_j \rangle \langle \phi_j | \psi \rangle \\ &= \sum_j \langle \psi | \hat{A} | \phi_j \rangle \langle \phi_j | \psi \rangle. \end{aligned} \tag{4.9}$$

Now we recognise the resolution of identity $\sum_j |\phi_j\rangle\langle\phi_j| = \mathbb{1}$ and thus we have

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle, \tag{4.10}$$

as expected.

4.2.3 Principle 4 ("state collapse postulate"):

Consider a system in the quantum state $|\psi\rangle$ on which a measurement of an observable A is performed. If the measurement yields the outcome a_j (an eigenvalue of $\hat{A}$), then the system is in the state $\frac{\hat{P}_j|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_j|\psi\rangle}}$ immediately after the measurement. Here $\hat{P}_j$ is the projection operator onto the subspace belonging to the eigenvalue a_j. For a non-degenerate eigenvalue with eigenvector $|\phi_j\rangle$ that is $\hat{P}_j = |\phi_j\rangle\langle\phi_j|$, which means the state afetr the measurement will be the state $\phi_j\rangle$.

Remark 22. In some ways principle 4 is a logical extension of principle 3: If we were to perform two measurements of the same observable instantly after one another, we would expect to obtain the same outcome in both with probability one.

Remark 23. Having the state collapse postulate in mind one often uses the formulation "to find a system in a state $|\phi\rangle$" in quantum mechanics. Such as for example in "... calculate the probability to find the system in the ground state.".

4.2.4 Principle 5 (dynamics):

The time-evolution of a quantum state $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$\mathrm{i}\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle, \tag{4.11}$$

where the operator $\hat{H}$ is the operator corresponding to the total energy of the system.

The solution of the Schrödinger equation can formally be written as

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle, \tag{4.12}$$

where $\hat{U}(t)$ is the *time-evolution operator*. For time independent Hamiltonians it is given by

$$\hat{U}(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}t\right). \tag{4.13}$$

Since the Hamiltonian $\hat{H}$ is Hermitian, the time-evolution operator $\hat{U}(t)$ is *unitary*. That is,

$$\hat{U}^{-1} = \hat{U}^\dagger. \tag{4.14}$$

Unitarity means that the inner product is conserved, i.e.

$$\langle\psi_1(t)|\psi_2(t)\rangle = \langle\psi_1(0)|\psi_2(0)\rangle, \tag{4.15}$$

with $|\psi_j(t)\rangle = \hat{U}(t)|\psi_j(0)\rangle$.

Remark 24. Think of "rotations on Hilbert space".

4.2.5 The method of stationary states in Dirac notation (for arbitrary Hilbert spaces)

Given: Hamiltonian $\hat{H}$, initial wave function $|\psi(t=0)\rangle$
Wanted: Wave function at time t, $|\psi(t)\rangle$

Method:

1. Calculate the eigenvalues E_n and normalised eigenstates $|\phi_n\rangle$ of the Hamiltonian $\hat{H}$.
2. Expand the initial wave function in the basis of eigenstates $\{|\phi_n\rangle\}$:

   $$|\psi(0)\rangle = \sum_n a_n|\phi_n\rangle.$$

   The coefficients are given by $a_n = \langle\phi_n|\psi(0)\rangle$.
3. The time evolution is then given by

   $$|\psi(t)\rangle = \sum_n a_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar}|\phi_n\rangle.$$

4.3 Commutators and uncertainties

The commutator of two observables restricts how accurately they can be measured simultaneously. In this chapter we shall discuss this in some detail. In this context we shall also learn about the famous *Heisenberg uncertainty principle*.

4.3.1 The uncertainty relations

The outcomes of many measurements of an observable A on identically prepared systems have a certain spread. The width of their distribution is characterised by the expectation value of the operator $(\hat{A} - \langle\hat{A}\rangle)^2$, that is, the *variance*

$$\begin{aligned}(\Delta A)^2 &:= \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle \\ &= \langle\hat{A}^2 - 2\langle\hat{A}\rangle\hat{A} + \langle\hat{A}\rangle^2\rangle \\ &= \langle\hat{A}^2\rangle - 2\langle\hat{A}\rangle^2 + \langle\hat{A}\rangle^2 \\ &= \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2.\end{aligned} \tag{4.16}$$

In quantum mechanics we refer to the *standard deviation*

$$\Delta A := \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}, \tag{4.17}$$

as *uncertainty* of A.

It follows from the principles of quantum mechanics that in general the product of the uncertainties of two observables cannot be arbitrarily small. Instead, it has a lower bound that is related to the commutator of the observables via the following

Theorem 6. *Consider the two Hermitian operators $\hat{A}$ and $\hat{B}$, with $[\hat{A},\hat{B}] \neq 0$. The product of the uncertainties of the observables A and B fulfils*

$$\Delta A \Delta B \geq \frac{1}{2}|\langle \hat{C} \rangle|, \tag{4.18}$$

where we have defined $\hat{C} := \mathrm{i}[\hat{A},\hat{B}]$.

Remark 25. The factor of i in the definition of $\hat{C}$ has been introduced such that $\hat{C}$ is Hermitian.

Proof. Let us shift the operators $\hat{A}$ and $\hat{B}$ such that their mean values are zero, that is, let us consider the operators

$$\hat{a} := \hat{A} - \langle \hat{A} \rangle, \quad \text{and} \quad \hat{b} := \hat{B} - \langle \hat{B} \rangle. \tag{4.19}$$

These operators have the same commutator as $\hat{A}$ and $\hat{B}$. That is,

$$[\hat{a},\hat{b}] = -\mathrm{i}\hat{C}. \tag{4.20}$$

Further we have

$$(\Delta A)^2 = \langle \hat{a}^2 \rangle \quad \text{and} \quad (\Delta B)^2 = \langle \hat{b}^2 \rangle. \tag{4.21}$$

Let us now consider the norm of the state $|\chi\rangle = (\hat{a} - \mathrm{i}\lambda\hat{b})|\psi\rangle$ for $\lambda \in \mathbb{R}$ and an arbitrary normalised state $|\psi\rangle$. We have

$$\begin{aligned} \langle \chi|\chi \rangle &= \langle \psi|(\hat{a} + \mathrm{i}\lambda\hat{b})(\hat{a} - \mathrm{i}\lambda\hat{b})|\psi\rangle \\ &= \langle (\hat{a} + \mathrm{i}\lambda\hat{b})(\hat{a} - \mathrm{i}\lambda\hat{b}) \rangle \\ &= \langle \hat{a}^2 + \lambda^2\hat{b}^2 + \mathrm{i}\lambda(\hat{b}\hat{a} - \hat{a}\hat{b}) \rangle \\ &= \langle \hat{a}^2 \rangle + \lambda^2\langle \hat{b}^2 \rangle + \mathrm{i}\lambda\langle \mathrm{i}\hat{C} \rangle \\ &= \langle \hat{a}^2 \rangle + \lambda^2\langle \hat{b}^2 \rangle - \lambda\langle \hat{C} \rangle \end{aligned} \tag{4.22}$$

On the other hand, we know that $\langle \chi|\chi \rangle \geq 0$. That is, we have

$$\langle \hat{a}^2 \rangle + \lambda^2\langle \hat{b}^2 \rangle - \lambda\langle \hat{C} \rangle \geq 0, \tag{4.23}$$

for all values of $\lambda \in \mathbb{R}$. Let us now evaluate for which value of λ the norm $\langle \chi|\chi \rangle$ becomes minimal. The location of the minimum is found where

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle \chi|\chi \rangle = 2\langle \hat{b}^2 \rangle\lambda - \langle \hat{C} \rangle = 0, \tag{4.24}$$

that is

$$\lambda = \frac{\langle \hat{C} \rangle}{2\langle \hat{b}^2 \rangle}. \tag{4.25}$$

(Note that this cannot be a maximum, since the function in (4.23) is a quadratic and goes to infinity at $\lambda \to \pm\infty$, and thus has a single minimum at a finite value of λ.) Reinserting this into the condition $\langle \chi|\chi \rangle_{min} \geq 0$ yields

$$\begin{aligned} \langle \chi|\chi \rangle_{min} &= \langle \hat{a}^2 \rangle + \frac{\langle \hat{C} \rangle^2}{4\langle \hat{b}^2 \rangle^2}\langle \hat{b}^2 \rangle - \frac{\langle \hat{C} \rangle^2}{2\langle \hat{b}^2 \rangle} \\ &= \langle \hat{a}^2 \rangle - \frac{\langle \hat{C} \rangle^2}{4\langle \hat{b}^2 \rangle} \geq 0, \end{aligned} \tag{4.26}$$

that is

$$(\Delta A)^2 \geq \frac{\langle \hat{C} \rangle^2}{4(\Delta B)^2}, \tag{4.27}$$

or

$$(\Delta A)(\Delta B) \geq \frac{|\langle \hat{C} \rangle|}{2}. \qquad \square$$

The special case of the uncertainty relation in theorem 6 for the case of position and momentum operator is known as *Heisenberg's uncertainty relation*:

$$\Delta p \Delta x \geq \frac{\hbar}{2}. \tag{4.28}$$

This means that one can never know the exact values of both position and momentum simultaneously.

Remark 26. The uncertainty relation gives a *lower* bound. There are states for which the actual uncertainty product for position and momentum for example is much larger than $\hbar$.

4.3.2 Commuting observables

If two observables commute they are in principle simultaneously measurable, according to the uncertainty relation. This is an aspect of the following

Theorem 7. *Commuting operators* $[\hat{A}, \hat{B}] = 0$ *posess a set of common eigenvectors.*

Exercise 7. Prove theorem 7 for the case of non-degenerate eigenvalues. I.e., consider an eigenvector $|\phi\rangle$ of $\hat{A}$ belonging to the eigenvalue $a \in \mathbb{R}$, that is $\hat{A}|\phi\rangle = a|\phi\rangle$, and show that $|\phi\rangle$ is also an eigenvector of $\hat{B}$ if $[\hat{A}, \hat{B}] = 0$.

Remark 27. If the eigenvalue a is degenerate (that is, it is a multiple eigenvalue), we can find a linear superposition of the corresponding eigenvectors that is an eigenvector of $\hat{B}$.

Remember that if we measure an observable A, after the measurement the quantum state of the system will have collapsed into the eigenspace of the operator $\hat{A}$ belonging to the eigenvalue that had been measured. Now if we measure an observable $\hat{B}$ directly afterwards that measurement will project the state of the system onto an eigenspace of $\hat{B}$. That means, only if $\hat{A}$ and $\hat{B}$ share eigenvectors, will the measurements be *compatible*, i.e. the measurement of one of the observables won't *delete* the information about the value of the first observable. Commuting operators have a set of shared eigenvectors, so they can be measured *simultaneously* or without the order of measurement changing the probabilities of the outcomes.

4.3.3 Complete set of commuting observables

Consider a set of Hermitian operators $\hat{A}_{1,2,\ldots}$ on a Hilbert space $\mathcal{H}$. Their simultaneous eigenvectors form a basis of $\mathcal{H}$. They are called a *complete set of commuting observables* if their eigenvalues uniquely define each basis vector (up to a phase).

If an operator $\hat{A}$ has only non-degenerate eigenvalues it is already a complete set of commuting observables on its own. If one or more eigenvalues is/are degenerate one can find a commuting operator to lift, or partially lift the degeneracy, and add further such operators to lift the degeneracies still present in this pair, and so on, until one arrives at a complete set of observables.

Let us consider a simple example for a three dimensional Hilbert space first. The operator

$$\hat{A} = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix}, \tag{4.29}$$

with $a_j \in \mathbb{R}$, is clearly Hermitian, and indeed its eigenvectors are the standard vectors e_j, which are a basis of $\mathbb{C}^3$, and could be uniquely labeled here by the eigenvalues of $\hat{A}$, i.e. e_j is the eigenvector of

$\hat{A}$ belonging to the eigenvalue a_j. If, however, some of the eigenvalues were degenerate, for example $a_2 = a_1$, or, for clarity, let's consider another operator $\hat{B}$

$$\hat{B} = \begin{pmatrix} b_1 & 0 & 0 \\ 0 & b_1 & 0 \\ 0 & 0 & b_2 \end{pmatrix}, \tag{4.30}$$

the situation would be different. We can still find a set of eigenvectors that are an orthogonal basis for $\mathbb{C}^3$, for example still the standard vectors e_j, or alternatively the vector e_3 and two orthogonal linear combinations of e_1 and e_2. However, these basis vectors cannot be uniquely identified by the corresponding eigenvalues of $\hat{B}$, as both e_1 and e_2 belong to the same eigenvalue b_1. If we in addition consider the operator

$$\hat{C} = \begin{pmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_2 \end{pmatrix}, \tag{4.31}$$

then the eigenvalues of $\hat{C}$ alone would also not be sufficient to identify the basis vectors, but those of $\hat{B}$ and $\hat{C}$ together would be. In the case here we could label the basis as

$$(b_1, c_1) \leftrightarrow e_1, \quad (b_1, c_2) \leftrightarrow e_2, \quad (b_2, c_2) \leftrightarrow e_3. \tag{4.32}$$

In infinite-dimensional Hilbert spaces it can be rather useful to have an abstract basis labelled according to the eigenvalues of an important observable (for example the energy), and if this has degenerate eigenvalues, it is useful to identify further commuting observables to uniquely label a basis of the Hilbert space. We will come back to this in more concrete physical examples later in the course.

Chapter 5

The harmonic oscillator

Let us now consider the quantum harmonic oscillator, the classical version of which we have studied in 1.2. Similarly to the classical case, the Hamiltonian is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2. \tag{5.1}$$

We want to solve the eigenvalue equation $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$. First of all we want to deduce the eigenvalues.

Remark 28. One way of solving this problem would be to express the eigenvalue equation in the Schrödinger formulation as $-\frac{\hbar^2}{2m}\frac{\partial^2\phi_E(x)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\phi_E(x) = E\phi_E(x)$, and determine for which values of E this has bound state solutions that fulfil $\phi_E(x \to \pm\infty) \to 0$. Here, however, we use another method that does not require us to solve any differential equation, and instead uses only uses algebraic arguments, based in the commutation relation of $\hat{q}$ and $\hat{p}$. .

5.1 Algebraic solution of the eigenvalue equation

Let us first introduce the dimensionless operators

$$\hat{Q} = \sqrt{\frac{m\omega}{\hbar}}\,\hat{q}, \quad \text{and} \quad \hat{\mathrm{P}} = \sqrt{\frac{1}{\mathrm{m}\omega\hbar}}\,\hat{\mathrm{p}}. \tag{5.2}$$

They fulfil the commutation relation

$$[\hat{Q}, \hat{P}] = \frac{1}{\hbar}[\hat{q}, \hat{p}] = \mathrm{i}\hat{I}. \tag{5.3}$$

In terms of these rescaled operators the Hamiltonian takes the form

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{P}^2 + \hat{Q}^2\right). \tag{5.4}$$

Now we introduce the operator

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\hat{Q} + \mathrm{i}\hat{P}\right), \tag{5.5}$$

and its adjoint operator

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{Q} - \mathrm{i}\hat{P}\right). \tag{5.6}$$

These operators fulfil the commutation relation

$$[\hat{a}, \hat{a}^\dagger] = \hat{I}. \tag{5.7}$$

Exercise 8. Verify the commutation relation (5.7) using the commutator(5.3), and rewrite the Hamiltonian in terms of $\hat{a}$ and $\hat{a}^\dagger$.

In terms of $\hat{a}$ and $\hat{a}^\dagger$ the Hamiltonian becomes

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}). \tag{5.8}$$

That is, we need to analyse the spectrum of the Hermitian operator $\hat{N} := \hat{a}^\dagger\hat{a}$.

Theorem 8. *$\hat{N}$ has a discrete spectrum consisting of the non-negative integers.*

To prove this theorem we will need the commutators $[\hat{N}, \hat{a}]$ and $[\hat{N}, \hat{a}^\dagger]$, which follow from $[\hat{a}, \hat{a}^\dagger] = 1$, as

$$\begin{aligned}[\hat{N}, \hat{a}] &= [\hat{a}^\dagger\hat{a}, \hat{a}] \\ &= [\hat{a}^\dagger, \hat{a}]\hat{a} \\ &= -[\hat{a}, \hat{a}^\dagger]\hat{a} \\ &= -\hat{a}\end{aligned} \tag{5.9}$$

and similarly,

$$\begin{aligned}[\hat{N}, \hat{a}^\dagger] &= \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] \\ &= \hat{a}^\dagger.\end{aligned} \tag{5.10}$$

Lemma 1. *The eigenvalues of $\hat{N}$ are non-negative. Further, if ν is an eigenvalue of $\hat{N}$ with eigenvector $|\nu\rangle$ then $\hat{a}|\nu\rangle$ is the zero vector if and only if $\nu = 0$.*

Proof. Consider an eigenstate $|\nu\rangle$ of $\hat{N}$ with eigenvalue ν, that is $\hat{N}|\nu\rangle = \nu|\nu\rangle$. Consider now the norm of the vector $\hat{a}|\nu\rangle$. We have

$$\begin{aligned}||\hat{a}|\nu\rangle||^2 &\geq 0 \\ \langle\nu|\hat{a}^\dagger\hat{a}|\nu\rangle &\geq 0 \\ \langle\nu|\hat{N}|\nu\rangle &\geq 0 \\ \nu\langle\nu|\nu\rangle &\geq 0,\end{aligned} \tag{5.11}$$

from which it follows that $\nu \geq 0$. □

Further, for $\nu = 0$ we have that $||\hat{a}|\nu\rangle||^2 = 0$, which means that $\hat{a}|0\rangle$ is the zero vector, we write $\hat{a}|0\rangle = 0$. (Note that $|0\rangle$ is *not* the zero vector here, it is simply a vector labelled by the index 0.) Also note that $\hat{a}|\nu\rangle$ can be the zero vector for no other value of ν according to equation (5.11).

Lemma 2. *If $|\nu\rangle$ is an eigenvector of $\hat{N}$ corresponding to the eigenvalue ν, and $\hat{a}|\nu\rangle \neq 0$, then $\hat{a}|\nu\rangle$ is also an eigenvector of $\hat{N}$ corresponding to the eigenvalue $\nu - 1$.*

Proof.

$$\begin{aligned}\hat{N}\hat{a}|\nu\rangle &= \left(\hat{N}\hat{a} - \hat{a}\hat{N} + \hat{a}\hat{N}\right)|\nu\rangle \\ &= \left([\hat{N}, \hat{a}] + \hat{a}\hat{N}\right)|\nu\rangle \\ &= \left(-\hat{a} + \hat{a}\hat{N}\right)|\nu\rangle \\ &= \hat{a}(\hat{N} - 1)|\nu\rangle \\ &= (\nu - 1)\hat{a}|\nu\rangle.\end{aligned} \tag{5.12}$$

□

Combining Lemma 1 and 2 we conclude that either the spectrum is empty (i.e. there are no eigenvalues at all) or $\nu = 0$ has to be in the spectrum, and no non-integer value of ν could possibly be in the spectrum (to guarantee that the series ν, $\nu - 1$, $\nu - 2, \ldots$ does not continue to negative values).

Lemma 3. *If $|\nu\rangle$ is an eigenvector of $\hat{N}$ corresponding to the eigenvalue ν, then $\hat{a}^\dagger|\nu\rangle$ is also an eigenvector of $\hat{N}$ corresponding to the eigenvalue $\nu + 1$.*

Exercise 9. Prove Lemma 3.

What we have shown now is that $\nu = 0$ *could be* an eigenvalue of $\hat{N}$. If it is, then starting from $\nu = 0$ via consecutive application of $\hat{a}^\dagger$ we thus deduce that all integers are eigenvalues of $\hat{N}$. If $\nu = 0$ is not an eigenvalue, the operator $\hat{N}$ has no eigenvalues at all. Thus, there is a *representation* of the algebra consisting of $\hat{a}, \hat{a}^\dagger$ and $\hat{N}$ (and the identity) in which $\hat{N}$ is an infinite-dimensional matrix with diagonal elements given by its eigenvalues, the non-negative integers. This completes our proof of Theorem 8.

The spectrum of the harmonic oscillator (Hamiltonian) thus consists of the discrete set of numbers $E_n = \hbar\omega(n + \frac{1}{2})$ where n is a non-negative integer,

$$\hat{H}|n\rangle = \hbar\omega(n + \tfrac{1}{2})|n\rangle. \tag{5.13}$$

Remark 29. The quantum energies are *quantised*. A classical particle in a harmonic oscillator potential can have any energy that is larger than the minimum of the potential (zero, in the present case), a quantum particle can only be in a superposition of states with discrete energies. Remembering the quantum rules in Chapter 4, this means that every time the energy of a quantum particle is measured, the outcome can only be one of the discrete energy eigenvalues. The expectation value resulting from a number of measurements, of course, can be any number larger than the smallest eigenvalue (which is larger than zero!), depending on the state of the particle (similar to the classical case).

Remark 30. The operators $\hat{a}$ and $\hat{a}^\dagger$ are often referred to as *ladder operators*, more specifically $\hat{a}$ is the *lowering* and $\hat{a}^\dagger$ the *raising* operator. Often one also referes to $\hat{a}$ as *annihilation* and $\hat{a}^\dagger$ as *creation* operator. The operator $\hat{N}$ is called the *number* operator.

5.2 Normalised eigenvectors

We will first consider a possible degeneracy of the eigenvalues. We will show that if the ground state is non-degenerate (which we will explicitly show in a later Chapter), then all the eigenvalues are non-degenerate, i.e. there is a unique (up to a complex factor) eigenvector $|n\rangle$ for each eigenvalue n. We shall now prove that if the eigenvalue n is non-degenerate so is the eigenvalue $n + 1$. Let us prove this by contradiction.

Assume that the eigenvalue n is non-degenerate, but there are two linearly independent eigenstates $|\phi_{n+1}\rangle$ and $|\chi_{n+1}\rangle$ belonging to the eigenvalue $n+1$. Applying the lowering operator to these two states we can produce the states $|\phi_n\rangle = \hat{a}|\phi_{n+1}\rangle$ and $|\chi_n\rangle = \hat{a}|\chi_{n+1}\rangle$. Now, since the eigenvalue n is non-degenerate these two vectors have to be multiples of each other, i.e. there exists a $\lambda \in \mathbb{C}$ such that

$$|\phi_n\rangle = \lambda|\chi_n\rangle. \tag{5.14}$$

Now acting on this relation with the raising operator $\hat{a}^\dagger$ yields:

$$\hat{a}^\dagger|\phi_n\rangle = \hat{a}^\dagger\hat{a}|\phi_{n+1}\rangle = \hat{N}|\phi_{n+1}\rangle = \lambda\hat{a}^\dagger|\chi_n\rangle = \lambda\hat{a}^\dagger\hat{a}|\chi_{n+1}\rangle = \lambda\hat{N}|\chi_{n+1}\rangle, \tag{5.15}$$

that is $\hat{N}|\phi_{n+1}\rangle = \lambda\hat{N}|\chi_{n+1}\rangle$. But since $|\phi_{n+1}\rangle$ and $|\chi_{n+1}\rangle$ are eigenstates of $\hat{N}$ with eigenvalue $(n + 1)$, we have

$$|\phi_{n+1}\rangle = \lambda|\chi_{n+1}\rangle, \tag{5.16}$$

which means the two assumed to be linearly independent eigenvectors are linearly dependent after all, and the eigenvalue $n+1$ is also non-degenerate. Thus, assuming that the eigenvalue $n=0$ is non-degenerate, we have shown that the eigenvalues are non-degenerate. □

We know that $\hat{a}^\dagger|n\rangle = c_n|n+1\rangle$. Let us now deduce the constants c_n assuming that the eigenvectors are normalised. We consider the norm of $|n+1\rangle$:

$$\langle n+1|n+1\rangle = \frac{1}{|c_n|^2}\langle n|\hat{a}\hat{a}^\dagger|n\rangle = \frac{1}{|c_n|^2}\langle n|\hat{N}+1|n\rangle = \frac{n+1}{|c_n|^2}\langle n|n\rangle. \tag{5.17}$$

Thus, if $|n\rangle$ is normalised, so is $|n+1\rangle$ for the choice $c_n = \sqrt{n+1}$. That is,

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{5.18}$$

from which it follows that

$$|n\rangle = \frac{1}{\sqrt{n!}}\hat{a}^{\dagger n}|0\rangle. \tag{5.19}$$

Remark 31. The corresponding equation to (5.18) for $\hat{a}$ is

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \tag{5.20}$$

5.3 Matrix representations in the harmonic oscillator basis

1. **Matrix representation of $\hat{a}^\dagger$:** From equation (5.18) it follows for the matrix elements of $\hat{a}^\dagger$ in the harmonic oscillator basis:

$$\langle m|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,\delta_{m,n+1}. \tag{5.21}$$

2. **Matrix representation of $\hat{a}$:** We can deduce the matrix elements for $\hat{a}$ either directly from equation (5.20) or from the fact that $\hat{a}$ is the adjoint of $\hat{a}^\dagger$, and thus their matrix elements are related by

$$\langle m|\hat{a}|n\rangle = \overline{\langle n|\hat{a}^\dagger|m\rangle}. \tag{5.22}$$

   From the matrix elements of $\hat{a}^\dagger$ we thus find the matrix elements of $\hat{a}$ as

$$\langle m|\hat{a}|n\rangle = \sqrt{n}\,\delta_{m,n-1} \tag{5.23}$$

3. **Matrix representation of $\hat{H}$:** The Hamiltonian matrix is diagonal in the eigenbasis, with diagonal elements

$$\langle m|\hat{H}|n\rangle = \hbar\omega(n+\frac{1}{2})\,\delta_{m,n} \tag{5.24}$$

Exercise 10. Matrix representation of $\hat{x}$ and $\hat{p}$.

(a) What are the matrix elements of the operators $\hat{q}$ and $\hat{p}$ in the basis of harmonic oscillator eigenstates $\{|n\rangle\}$?

(b) Verify that these matrices fulfil the correct commutation relation.

5.4 Harmonic oscillator basis - A simple numerical method for general potentials

The matrix representation of position and momentum operator in the harmonic oscillator basis forms the basis of a simple numerical method to calculate eigenvalues of one-dimensional systems with Hamiltonians that are functions of position and momentum operators. Here the matrices are terminated at finite size, leading to an approximation. For more details on this method see H. J. Korsch and M. Glück, *Computing quantum eigenvalues made easy*, Eur. J. Phys. **23**, 413 (2002).

The following matlab program gives out the 8 lowest energy states of the harmonic oscillator Hamiltonian $\hat{H} = \hat{p}^2/2 + \hat{x}^2/2$:

```
clear all
N=100; %matrix size

%matrices for postition and momentum operators
n=1:N-1;
k=sqrt(n);

Q=sqrt(0.5)*(diag(k,1)+diag(k,-1));
P=i*sqrt(0.5)*(diag(k,-1)-diag(k,1)):

%Hamiltonian
H=0.5*P^2+0.5*Q^2;

%eigenvalues
EigSort=sort(eig(H));
EigSort(1:8)
```

This programme can be modified to calculate the spectrum of many other Hamiltonians with different potential functions. In a video I discuss the example of a quadratic potential with a small quartic contribution $V(x) = x^2 + cx^4$.

Chapter 6

Representations

In this chapter, we finally connect the abstract formulation of quantum mechanics expressed in the five principles, and using the Dirac notation, back to the Schrödinger wave formulation we have encountered in Chapter 2. The essence is that in Schrödinger's wave mechanics, the position plays the role of a preferred observable, and the wave function is nothing but the state of the quantum system, expressed in the basis of eigenstates of the position operator. What complicates the matter, is that the position operator has a continuous spectrum, and no normalisable eigenfunctions on the Hilbert space, which leads to some technical complications when formulating the theory.

6.1 Discrete and continuous spectra - normalisable and *improper* eigenvectors

Consider a linear operator $\hat{A}$ acting on a complex Hilbert space $\mathcal{H}$. If there exists a pair of a complex number $\lambda \in \mathbb{C}$ and a non-zero vector $|\phi\rangle \in \mathcal{H}$, such that

$$\hat{A}|\phi\rangle = \lambda|\phi\rangle, \tag{6.1}$$

then $|\phi\rangle$ is an *eigenvector* of $\hat{A}$ belonging to the *eigenvalue* λ.

We will now follow Dirac's argument, to argue why eigenvectors with a continuous set of eigenvalues cannot be normalisable. There are more rigorous mathematical treatments of this problem, which are covered in advanced analysis lectures. Here we stay within the realm of quantum mechanics, and assume that the principles of Chapter 4 should be applicable even to an observable with a continuous spectrum, or else such observables would not be permissible in QM. A central idea in the principles of QM is that the eigenstates of an observable form a basis of the relevant Hilbert space, i.e. for discrete eigenvalues λ_n belonging to eigenvectors $|\phi_n\rangle$, or more generally for potentially degenerate eigenvalues, belonging to eigenspaces with projectors $\hat{P}_n$, an arbitrary vector in the Hilbert space can be expanded as

$$|\psi\rangle = \sum_n \hat{P}_n|\psi\rangle. \tag{6.2}$$

Now, let us consider the case of a continuous spectrum. For simplicity, let us assume that the eigenvalues form a continuous interval on the real line $[a, b] \subset \mathbb{R}$. The equivalent of equation (6.2) then states that every vector $|\psi\rangle$ can be written as

$$|\psi\rangle = \int_a^b \hat{P}_\lambda|\psi\rangle \mathrm{d}\lambda, \tag{6.3}$$

however, this implies that the norm of the eigenvectors cannot be finite. Let us for simplicity assume that the spectrum is non-degenerate, and write

$$|\psi\rangle = \int_a^b \langle\phi_\lambda|\psi\rangle|\phi_\lambda\rangle \mathrm{d}\lambda, \tag{6.4}$$

If we consider a single eigenvector $|\phi_\lambda\rangle$ we have

$$|\phi_\lambda\rangle = \int_a^b \langle\phi_{\lambda'}|\phi_\lambda\rangle|\phi_{\lambda'}\rangle \mathrm{d}\lambda'. \tag{6.5}$$

Now, since $\hat{A}$ is a self-adjoint operator, the eigenvectors belonging to different eigenvalues are orthogonal to each other, meaning that the integrand vanishes at all but one point $\lambda = \lambda'$. The only way to make the equality work is to assume that the squared norm $\langle\phi_\lambda|\phi_\lambda\rangle$ of an eigenvector belonging to an eigenvalue in the continuous spectrum is infinite. Specifically, we need

$$\langle\phi_{\lambda'}|\phi_\lambda\rangle = \delta(\lambda' - \lambda), \tag{6.6}$$

where $\delta(x)$ denotes the Dirac Delta-Distribution, which is infinite at $\lambda = \lambda'$, which means that an eigenvalue in the continuum is not strictly speaking an eigenvalue, since it does not have an eigenvector in the Hilbert space.

Remark 32. Remember that a Hilbert space is a complete metric space, that is, it cannot have elements with infinite norm.

Remark 33. The continuous "eigenvalues" are referred to simply as *the continuous spectrum* in mathematics, and together with the discrete eigenvalues they make up the whole spectrum of a self-adjoint operator. Sometimes they are referred to as *improper* or *approximate* eigenvalues, and the corresponding "eigenvectors" (with infinite norm) are referred to as *improper* eigenvectors.

Mathematically, the continuous spectrum is defined using a generalisation of the eigenvalue equation, that circumvents the concept of eigenvectors. The eigenvalue equation (6.1) implies that

$$(\hat{A} - \lambda\hat{I})|\phi\rangle = 0, \tag{6.7}$$

i.e., the operator $(\hat{A} - \lambda\hat{I})$ is not invertible when λ is an eigenvalue. Bounded Hermitian operators $\hat{A}$ have discrete real eigenvalues (forming what is known as the *point spectrum*). Unbounded Hermitian operators, however, might have an (additional) *continuous spectrum*, consisting of values $\lambda \in \mathbb{R}$ that span a continuous interval, and for which the operator $(\hat{A} - \lambda\hat{I})^{-1}$ is defined, however, its domain is not the whole Hilbert space. As we have seen, there are no eigenvectors in the Hilbert space, corresponding to these values of λ, but one can extend the notion of eigenvectors to vectors with an infinite norm in the sense explained above.

In quantum mechanics, we simply refer to the continuous spectrum as eigenvalues and use the same bra-ket notation for the improper eigenvectors as for the normalisable ones, belonging to discrete eigenvalues. With the only difference that for eigenvectors belonging to discrete eigenvalues λ_n we have

$$\langle\phi_n|\phi_m\rangle = \delta_{n,m}, \tag{6.8}$$

while for continuous eigenvalues this is replaced by (6.6).

Importantly, while the eigenvectors of an operator $\hat{A}$ with a purely discrete spectrum provide a resolution of the identity as

$$\sum_n |\phi_n\rangle\langle\phi_n| = \hat{I}, \tag{6.9}$$

the eigenvectors of an operator with a purely continuous spectrum fulfil

$$\int_a^b |\phi_\lambda\rangle\langle\phi_\lambda| \mathrm{d}\lambda = \hat{I}. \tag{6.10}$$

6.1.1 A few comments on the Dirac δ-Distribution

The δ-distribution is strictly speaking only defined inside an integral, and fulfils the important property

$$\int_{-\infty}^{\infty} f(x)\delta(x)\mathrm{d}x = f(0), \tag{6.11}$$

for functions $f(x)$ with compact support on $\mathbb{R}$.

The δ-distribution can be expressed as the limit of various well-defined functions, for example as the limit of a Gaussian with vanishing width,

$$\delta(x) = \lim_{\sigma\to 0} \tfrac{1}{\sigma\sqrt{2\pi}} \mathrm{e}^{-\frac{x^2}{2\sigma^2}}, \tag{6.12}$$

or as the Fourier transform of a plane wave as

$$\delta(x-\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ik(x-\alpha)} dk. \tag{6.13}$$

Remark 34. In equation (6.12) we have yet another abuse of notation. Writing $\delta(x) = g(x)$ is a short-hand form for the slightly more rigorous statement $\int_{-\infty}^{\infty} f(x)\delta(x)\mathrm{d}x = \int_{-\infty}^{\infty} f(x)g(x)\mathrm{d}x$.

6.2 Eigenvalues of the position operator

While there are no finite dimensional matrices $\hat{q}$ and $\hat{p}$ that fulfil the required commutation relation $[\hat{q},\hat{p}] = \mathrm{i}\hbar\hat{I}$ for position and momentum operators, we have seen in Chapter 5 that there are infinite dimensional matrices (in the harmonic oscillator basis), with the elements

$$\langle m|\hat{q}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right), \tag{6.14}$$

and

$$\langle m|\hat{p}|n\rangle = \mathrm{i}\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}\right). \tag{6.15}$$

Let us now formally solve the eigenvalue equation for this infinite dimensional matrix representation of $\hat{q}$. Defining the length $L = \sqrt{\frac{\hbar}{m\omega}}$, $\hat{q}$ has the matrix representation

$$Q = \frac{L}{\sqrt{2}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \ddots \\ \vdots & \vdots & & \ddots & \ddots \end{pmatrix} \tag{6.16}$$

in the harmonic oscillator basis. The eigenvalue equation

$$\hat{q}|\phi_\lambda\rangle = \lambda|\phi_\lambda\rangle \tag{6.17}$$

translates into a recursion relation for the components $\phi_n(\lambda) := \langle n|\phi_\lambda\rangle$ of the eigenvector in the harmonic oscillator basis, with

$$\phi_1(\lambda) = \frac{\lambda\sqrt{2}}{L}\phi_0(\lambda) \tag{6.18}$$

and

$$\sqrt{n}\phi_{n-1}(\lambda) + \sqrt{n+1}\phi_{n+1}(\lambda) = \frac{\lambda\sqrt{2}}{L}\phi_n(\lambda), \quad \text{for} \quad n > 0. \tag{6.19}$$

That is, fixing the first component ϕ_0 arbitrarily, we can always construct the other components of an eigenvector, corresponding to any real eigenvalue λ. These vectors, however, will not be normalisable. To solve the recursion relation for the eigenvector components, we recognise it as a version of the recursion relation fulfilled by the *Hermite polynomials* $H_n(x)$, which are a family of orthogonal polynomials, fulfilling the orthogonality relation

$$\int_{-\infty}^{+\infty} H_m(x)H_n(x)\mathrm{e}^{-x^2}\mathrm{d}x = \sqrt{\pi}2^n n!\delta_{m,n}. \tag{6.20}$$

They can be defined via the expression

$$\mathrm{H}_n(x) = \mathrm{e}^{x^2/2}\left(x - \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \mathrm{e}^{-x^2/2}. \tag{6.21}$$

They are polynomials of degree n with alternating parity (even, odd, even, ...). Importantly, they fulfil the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x),$$

with $H_0(x) = 1$, and $H_1(x) = 2x$.

We notice the similarity to the recursion relation (6.19). Starting from (6.19), let us introduce the rescaled components $\chi_n(\lambda)$ of the eigenvector as

$$\chi_n(\lambda) = \sqrt{2^n\, n!}\phi_n(\lambda). \tag{6.22}$$

After a little algebra we find that these fulfil the recursion relation

$$\chi_{n+1}(\lambda) = 2\frac{\lambda}{L}\chi_n(\lambda) - 2n\chi_{n-1}(\lambda), \tag{6.23}$$

and thus we have

$$\chi_n(\lambda) \propto H_n(\frac{\lambda}{L}), \tag{6.24}$$

and thus

$$\phi_n(\lambda) = \frac{\phi_0(\lambda)}{\sqrt{2^n\, n!}}H_n(\frac{\lambda}{L}). \tag{6.25}$$

However, as we expect, these eigenvectors are not normalisable. We have

$$\langle\phi(\lambda)|\phi(\lambda)\rangle = \sum_{n=0}^{\infty}\frac{|\phi_0(\lambda)|^2}{2^n\, n!}H_n^2(\lambda/L), \tag{6.26}$$

which, unfortunately, is a divergent series.

Of course, from the discussions in section 6.1 we already know that we expect (with the correct "normalising" factor) $\langle\phi(\lambda)|\phi(\lambda')\rangle = \delta(\lambda - \lambda')$. This indeed can be seen from the properties of the Hermite polynomials in a suitable limit. The Hermite polynomials fulfil the important relation (also known as Mehler's formula)

$$\sum_{n=0}^{\infty}\frac{H_n(x)H_n(y)}{n!}\left(\frac{c}{2}\right)^n = \frac{1}{\sqrt{1-c^2}}\mathrm{e}^{-\frac{c^2(x^2+y^2)-2cxy}{1-c^2}}, \quad \text{for} \quad -1 < c < 1. \tag{6.27}$$

Choosing $\phi_0(\lambda) = \frac{1}{\pi^{1/4}\sqrt{L}}\mathrm{e}^{-\frac{\lambda^2}{2L^2}}$, we thus have

$$\langle\phi(\lambda)|\phi(\lambda')\rangle = \frac{1}{L\sqrt{\pi}}\mathrm{e}^{-\frac{(\lambda'^2+\lambda^2)}{2L^2}}\lim_{c\to 1}\frac{1}{\sqrt{1-c^2}}\mathrm{e}^{-\frac{c^2(\lambda^2+\lambda'^2)-2c\lambda\lambda'}{(1-c^2)L^2}}, \tag{6.28}$$

$$\tag{6.29}$$

the overall exponent can be rewritten as

$$-\frac{(\lambda'^2+\lambda^2)}{2L^2} - \frac{c^2(\lambda^2+\lambda'^2)-2c\lambda\lambda' y}{(1-c^2)L^2} = -\frac{(1-c)(\lambda+\lambda')^2}{4(1+c)L} - \frac{(1+c)^2(\lambda-\lambda')^2}{4(1-c^2)L^2}, \tag{6.30}$$

which simplifies our expression to

$$\langle\phi(\lambda)|\phi(\lambda')\rangle = \frac{1}{\sqrt{\pi}}\lim_{c\to 1}\frac{1}{L\sqrt{1-c^2}}\mathrm{e}^{-\frac{(\lambda-\lambda')^2}{(1-c^2)L^2}}, \tag{6.31}$$

$$\tag{6.32}$$

Introducing the variable $\sigma^2 = \frac{1-c^2}{2}$ we can rewrite this as

$$\langle\phi(\lambda)|\phi(\lambda')\rangle = \frac{1}{L}\lim_{\sigma\to 0}\frac{\mathrm{e}^{-\frac{1}{2\sigma^2}(\frac{\lambda}{L}-\frac{\lambda'}{L})^2}}{\sigma\sqrt{2\pi}}, \tag{6.33}$$

which is indeed one of the representations of the δ-distribution we have encountered in section 6.1, and using $\delta(ax) = \frac{1}{|a|}\delta(x)$ we thus have

$$\langle\phi(\lambda)|\phi(\lambda')\rangle = \delta(\lambda - \lambda'). \tag{6.34}$$

In summary, we have found that the position operator has a continuous spectrum spanning the whole real line $x \in \mathbb{R}$, with corresponding (generalised) eigenvectors $|x\rangle$,

$$\hat{q}|x\rangle = x|x\rangle. \tag{6.35}$$

The eigenvectors fulfil the continuous analogue of the orthonormality condition,

$$\langle x|x'\rangle = \delta(x - x'), \tag{6.36}$$

and form a resolution of the identity as

$$\int_{-\infty}^{+\infty} |x\rangle\langle x|\mathrm{d}x = \hat{I}. \tag{6.37}$$

6.3 Position representation

The wave function in position representation $\psi(x)$ corresponds to the coefficients of the abstract vector $|\psi\rangle$ in the basis of the eigenfunctions of $\hat{q}$, that is $\psi(x) := \langle x|\psi\rangle$, and

$$|\psi\rangle = \int_{-\infty}^{\infty} \psi(x)|x\rangle\mathrm{d}x. \tag{6.38}$$

The squared norm of the state $|\psi\rangle$ can thus be evaluated in position representation as

$$\langle\psi|\psi\rangle = \int_{-\infty}^{+\infty} |\psi(x)|^2\mathrm{dx}. \tag{6.39}$$

Demanding the norm to be finite, we thus identify our Hilbert space with the space of square integrable functions, $L^2(\mathbb{R})$.

The *matrix elements* of the position operator in the position basis are

$$\langle x|\hat{q}|x'\rangle = x\delta(x - x'), \tag{6.40}$$

which simply means that the position operator is diagonal in the basis of its eigenvectors, as expected. We can also define the position operator in the position representation directly by its action on a square integrable function $\psi(x) \in L^2$ as

$$\hat{q} : \psi(x) \mapsto x\psi(x). \tag{6.41}$$

More formally, this is equivalent to

$$\langle x|\hat{q}|\psi\rangle = x\langle x|\psi\rangle = x\psi(x). \tag{6.42}$$

When measuring a particle's position, according to principle 3, the probability of obtaining a value in the interval $I = [a, b]$ is given by $\int_a^b |\psi(x)|^2\mathrm{d}x$, as we have assumed in Chapter 2. That is, the interpretation of Schrödinger's wave function is a special case of principle 3.

With the definition of the position operator, also the *momentum operator* $\hat{p}$ is fixed, because $\hat{p}$ and $\hat{q}$ have to fulfil equation (4.1). The operator

$$\hat{p} : \psi(x) \mapsto -\mathrm{i}\hbar\frac{\partial}{\partial x}\psi(x) \tag{6.43}$$

fulfils this condition with (6.41).

Exercise 11. Verify that the operators (6.43) and (6.41) indeed fulfil the commutation relation (4.1), by applying their commutator onto a test function $\psi(x) \in L^2$.

Remark 35. One could in principle add an arbitrary function of $\hat{q}$ to $\hat{p}$ and still fulfil the commutation relation (4.1). The reason why it is fine to choose this function to be zero is a little subtle, and does not need to concern us here. If you are interested in the details, see e.g. Dirac's textbook.

Finally, the *kinetic energy* is described by $E_{kin} = \frac{p^2}{2m}$ in classical mechanics. This is analogous in quantum mechanics, and thus the operator of kinetic energy in the position representation is given by

$$\hat{E}_{kin} = \frac{\hat{p}^2}{2m} : \psi(x) \mapsto -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x). \tag{6.44}$$

With this we are back to Schrödinger's equation as it appears in wave mechanics, where the Hamiltonian for a particle in a one-dimensional potential is the operator $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$, and thus the Schrödinger equation in position representation,

$$\mathrm{i}\hbar\langle x|\dot{\psi}\rangle = \langle x|\hat{H}|\psi\rangle, \tag{6.45}$$

explicitly reads

$$\mathrm{i}\hbar\dot{\psi}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t). \tag{6.46}$$

6.4 Change of bases/representation

To change between two representations, we simply insert a resolution of the identity in the basis we are starting from. That is, for example, if we have the coefficients ψ_n of a vector $|\psi\rangle$ in the harmonic oscillator basis, that is, $\psi_n = \langle n|\psi\rangle$ and want to know its position representation $\psi(x) = \langle x|\psi\rangle$ we find this in the following way.

$$\psi(x) = \langle x|\psi\rangle = \langle x|\hat{I}|\psi\rangle = \langle x|\left(\sum_n |n\rangle\langle n|\right)|\psi\rangle \tag{6.47}$$

$$= \sum_n \langle x|n\rangle\langle n|\psi\rangle \tag{6.48}$$

$$= \sum_n \psi_n \phi_n(x), \tag{6.49}$$

where $\phi_n(x) = \langle x|n\rangle$ denotes the position representation of the harmonic oscillator eigenvector belonging to the eigenvalue $\hbar\omega(n + \frac{1}{2})$. As a second example, if we want to translate from the position representation $\psi(x) = \langle x|\psi\rangle$ to the momentum representation $\tilde{\psi}(p) = \langle p|\psi\rangle$, where $|p\rangle$ denotes the eigenstate of the momentum operator $\hat{p}$ belonging to the eigenvalue p, we find

$$\tilde{\psi}(p) = \langle p|\psi\rangle \tag{6.50}$$

$$= \int_{-\infty}^{+\infty} \langle p|x\rangle\langle x|\psi\rangle \mathrm{d}x \tag{6.51}$$

$$= \int_{-\infty}^{+\infty} \phi_p^*(x)\psi(x)\mathrm{d}x, \tag{6.52}$$

where $\phi_p(x) = \langle x|p\rangle$ denotes the position representation of the momentum eigenvector belonging to momentum p, which you can deduce from solving the eigenvalue equation for $\hat{p}$ in position representation.

Chapter 7

Spectral properties of one-dimensional quantum systems

In this chapter we will analyse the eigenvalues of the Hamiltonian for a number of important one-dimensional quantum systems. That is, we solve the time-independent Schrödinger equation. Again, we consider systems of the form $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$. Physically these Hamiltonians describe a particle (in one-dimensional space) of mass m under the influence of an external potential $V(x)$. This could be, for example, an electron in an atom, where the potential is given by the interaction with the nucleus and the other electrons (this is complicated and obviously three-dimensional and we will not discuss details in this chapter). The particle in a box is a good approximation for electrons in so-called *quantum dots*, which are fabricated semiconductor structures in which electrons are confined. Atoms in *optical potentials* (where quantum optical effects are used to confine atoms with laser setups) are another experimental system described by Hamiltonians of the form considered here. Experimentally these systems can often be made *quasi one-dimensional*. Similarly atoms can be trapped magnetically, in approximately harmonic traps described by quadratic potentials. There are countless other examples, even outside quantum physics: The Helmholtz equation for microwaves in flat (quasi two-dimensional) resonators is similar to the Schrödinger equation where the potential is related to the structure of the cavity. Similar analogies exist in optical setups.

7.1 Position representation of the harmonic oscillator eigenstates

With the position representation from Chapter 6 at hand, we can now return to the harmonic oscillator and provide the position representation of the eigenstates. In fact, we have already calculated this along the way when we considered the eigenvalues of the position operator in section 6.2, where we deduced that

$$\langle n|x\rangle = \frac{1}{\pi^{1/4}\sqrt{2^n\, n!}\sqrt{L}} \mathrm{e}^{-\frac{x^2}{2L^2}} H_n(\frac{x}{L}). \tag{7.1}$$

Thus, we have implicitly found there that

$$\phi_n(x) = \langle x|n\rangle = \frac{1}{\pi^{1/4}\sqrt{2^n\, n!}\sqrt{L}} \mathrm{e}^{-\frac{x^2}{2L^2}} H_n(\frac{x}{L}). \tag{7.2}$$

Nevertheless, let us, as an exercise also consider the problem in position representation picking up at an earlier point and verifying (7.2). Let us start with deducing the position representation of the ground state (the state belonging to the lowest eigenvalue, $E_0 = \frac{\hbar\omega}{2}$), directly from the condition $\hat{a}|0\rangle = 0$. This will also provide the direct verification of the statement that the ground state energy is not degenerate, which we had used without proof in Chapter 5. We can deduce the functional form of $\phi_0(x)$ from the equation $\hat{a}|0\rangle = 0$ in position representation.

First we remember the definition of $\hat{a}$ in terms of $\hat{q}$ and $\hat{p}$:

$$\hat{a} := \frac{1}{\sqrt{2}}\left(\hat{Q} + \mathrm{i}\hat{P}\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\hat{q} + \mathrm{i}\sqrt{\frac{1}{m\omega\hbar}}\hat{p}\right) \tag{7.3}$$

We recall the expressions for $\hat{q}$ and $\hat{p}$ in position representation,

$$\langle x|\hat{q}|\phi\rangle = x\phi(x), \quad \text{and} \quad \langle x|\hat{p}|\phi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\phi(x), \tag{7.4}$$

to find

$$\langle x|\hat{a}|\phi\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right)\phi(x). \tag{7.5}$$

Thus, the ground state wave function fulfils the condition

$$\frac{\partial}{\partial x}\phi_0(x) = -\frac{m\omega}{\hbar}x\phi_0(x). \tag{7.6}$$

Thus we find

$$\phi_0(x) = \phi_0(x) = c\,\mathrm{e}^{-\frac{m\omega}{2\hbar}x^2}, \qquad c \in \mathbb{C}. \tag{7.7}$$

We can deduce the normalisation constant c by requiring the wave function to be normalised. From

$$\int_{-\infty}^{\infty}|\phi_0(x)|^2\mathrm{d}x = \int_{-\infty}^{\infty}|c|^2\mathrm{e}^{-\frac{m\omega}{\hbar}x^2}\mathrm{d}x = 1, \tag{7.8}$$

we deduce

$$|c|^2 = \sqrt{\frac{m\omega}{\pi\hbar}}, \tag{7.9}$$

and thus we choose

$$c = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}, \tag{7.10}$$

such that the ground state wave function is normalised, real, and positive. In summary, we have found the position representation of the normalised ground state wave function of the operator $\hat{N}$ (and thus the harmonic oscillator):

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right). \tag{7.11}$$

We can now use the abstract expression for the chain of eigenvectors starting from the ground state in equation (5.19), to deduce the position representation of these eigenvectors, $\phi_n(x) := \langle x|n\rangle$. Using expression (5.19) we can deduce all $\phi_n(x)$ from $\phi_0(x)$. To find the position representations of the higher excited states, we need to apply $\hat{a}^\dagger$ onto the ground state:

$$\langle x|n\rangle = \phi_n(x) = \frac{1}{\sqrt{n!}}\langle x|(\hat{a}^\dagger)^n|0\rangle. \tag{7.12}$$

That is,

$$\begin{aligned}\phi_n(x) &= \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right)\right)^n\phi_0(x)\\ &= \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right)^n\exp\left(-\frac{m\omega}{2\hbar}x^2\right).\end{aligned} \tag{7.13}$$

Explicitly the $\phi_n(x)$ can be expressed in terms of Hermite polynomials $\mathrm{H}_n(x)$ as

$$\phi_n(q) = \sqrt{\frac{\sqrt{m\omega}}{2^n n!\sqrt{\pi\hbar}}}\,\mathrm{H}_n(q)\,\mathrm{e}^{-q^2/2}, \tag{7.14}$$

with $q = \sqrt{\frac{m\omega}{\hbar}}x$, as expected.

7.2 Properties of eigenfunctions for general one-dimensional potentials

There are only very few examples of Hamiltonian operators the spectrum of which can be deduced analytically. In general, approximative or numerical methods have to be applied. Yet, a few general remarks can be made about the solutions of time-independent Schrödinger equations of the form

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\phi_E(x)=E\phi_E(x):\tag{7.15}$$

- In general there are two types of solutions of (7.15) that we can interpret in a meaningful way in Schrödinger's wave mechanics: The bound states, for which $\phi(x\to\pm\infty)\to 0$, and the *continuum states*, which are improper eigenfunctions (not in L^2), belonging to eigenvalues in the continuous part of the spectrum.

- For potentials for which $V(x\to\pm\infty)\to\infty$ there are only bound states (i.e. only discrete eigenvalues - this is the *quantisation* part of quantum mechanics again - energies can often only have discrete values.)

- Eigenfunctions can be chosen real valued.

  Proof. Assume we have a complex solution $\phi(x)$ of the Schrödinger equation. Then also its complex conjugate function $\phi^*(x)$ is a solution. Thus, the linear combination $\phi(x)+\phi^*(x)$ is a real valued solution of the Schrödinger equation. □

- There are no bound states with eigenenergies smaller than the minimum of the potential.

  Proof. We have

  $$\frac{\partial^2\phi_E(x)}{\partial x^2}=\frac{2m}{\hbar^2}(V(x)-E)\phi_E(x).\tag{7.16}$$

  Now if $E<V_{min}(x)$ then the the wave function $\phi_E(x)$ and its second derivative would have the same sign for all x. That is if the wave function would have to curve away from the x-axis everywhere. Such a function however, can not be normalisable. □

- The expectation value of a Hamiltonian is bounded from below by the lowest energy eigenvalue.

  We will prove this in the end of the week lecture.

- The bound state eigenvalues are non-degenerate (that is, there is only one linearly independent solution per eigenvalue).

  Proof. Let us first rewrite the Schrödinger equation (7.15) in the form

  $$\phi''(x)+k^2(x)\phi(x)=0,\tag{7.17}$$

  where we have introduced the function $k=\sqrt{\frac{2m}{\hbar^2}(E-V(x))}$. Suppose now that $\phi_1(x)$ and $\phi_2(x)$ are two bound state eigenfunctions corresponding to the same energy E. We shall show now that this implies that $\phi_1(x)$ and $\phi_2(x)$ are linearly dependent, i.e. they differ at most by a multiplicative factor.

  We have

  $$\phi_j''(x)/\phi_j(x)=-k(x)^2,\tag{7.18}$$

  for $j=1,2$. That is,

  $$\phi_1''(x)/\phi_1(x)=\phi_2''(x)/\phi_2(x),\tag{7.19}$$

  or

  $$\phi_1''(x)\phi_2(x)-\phi_2''(x)\phi_1(x)=0.\tag{7.20}$$

We realise that the left hand side is equal to the derivative of $\phi_1'(x)\phi_2(x) - \phi_2'(x)\phi_1(x)$, that is we have

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\phi_1'(x)\phi_2(x) - \phi_2'(x)\phi_1(x)\right) = 0. \tag{7.21}$$

Integrating this yields

$$\phi_1'(x)\phi_2(x) - \phi_2'(x)\phi_1(x) = c, \qquad c \in \mathbb{C}. \tag{7.22}$$

Since we consider bound states we have that $\phi_j(x \to \infty) \to 0$ while the derivative stays bounded, and thus we deduce that $c = 0$. We now integrate the expression

$$\phi_1'(x)/\phi_1(x) = \phi_2'(x)/\phi_2(x), \tag{7.23}$$

to find

$$\ln \phi_1(x) = \ln \phi_2(x) + const. \tag{7.24}$$

that is

$$\phi_1(x) \propto \phi_2(x). \tag{7.25}$$

□

- The ground state (the state corresponding to the lowest energy eigenvalue) does not have zeros (apart from the asymptotic ones at $x \to \pm\infty$).
- The n-th excited state (the state corresponding to the $(n+1)$th eigenvalue) has n zeros inside the potential.

  For a hand-wavy explanation of this see for example Barton Zwiebach's video lecture on the topic.

7.2.1 Symmetric potentials - parity

Consider the Hermitian operator $\hat{S}$ on the Hilbert space of square integrable functions that interchanges x with $-x$, that is, $\hat{S}\psi(x) = \psi(-x)$. This is called the *parity* operator. The eigenfunctions of the parity operator fulfil

$$\hat{S}\phi_s(x) = \phi_s(-x) = s\phi_s(x). \tag{7.26}$$

On the other hand $\hat{S}^2 = \hat{I}$, that is,

$$\hat{S}(\hat{S}\phi_s(x)) = s^2\phi_s(x) = \phi_s(x). \tag{7.27}$$

Thus, we have $s^2 = 1$, and therefore the only two eigenvalues of the parity operator are

$$s = \pm 1. \tag{7.28}$$

The corresponding eigenfunctions are all even or odd functions $\phi_\pm(-x) = \pm\phi(x)$. (The parity operator is highly degenerate).

A Hamiltonian of the form $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ commutes with $\hat{S}$ if $V(x) = V(-x)$. This can be seen as follows. Consider the action of the commutator on a test function $\psi(x) \in L^2$:

$$\begin{aligned}[\hat{H}, \hat{S}]\psi(x) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(-x) + V(x)\psi(-x) \\ &\quad + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)^2}\psi(-x) - V(-x)\psi(-x) \\ &= V(x)\psi(-x) - V(-x)\psi(-x),\end{aligned} \tag{7.29}$$

which is zero for arbitrary wave functions $\psi(x)$ if and only if $V(-x) = V(x)$.

According to theorem 7, if the eigenvalues of $\hat{H}$ are non-degenerate, the corresponding eigenfunctions are either odd or even. Since the eigenvalues of one-dimensional Hamiltonians of the form $V(x \to \pm\infty) \to \infty$ (*binding potentials*) are always non-degenerate. If the potential is symmetric, the eigenfunctions are either even or odd. We have already seen an example when we discussed the particle in a square well in Chapter 2, there the potential was symmetric with respect to $x = \frac{L}{2}$ and the eigenfunctions were even and odd with respect to this point.

Remark 36. Unfortunately most of the statements above do not carry over to higher dimensional systems. This concerns in particular the non-degeneracy of eigenvalues and hence the symmetry of eigenfunctions in symmetric potentials.

7.3 Piecewise constant potentials

7.3.1 Piecewise constant potentials and boundary conditions

For the remainder of this chapter we are specifically looking for the solutions E and $\phi_E(x)$ of the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_E(x) + V(x)\phi_E(x) = E\phi_E(x), \tag{7.30}$$

where the potential $V(x)$ is piecewise constant. Rewriting this in the form

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_E(x) = (E - V(x))\phi_E(x), \tag{7.31}$$

emphasises that the second derivative of an eigenfunction is essentially proportional to the value of the potential energy. Thus, at values of x at which the potential makes a finite jump, so does the second derivative of the wave function, which means that the first derivative is continuous, while the wave function itself is continuous and continuously differentiable. If the potential makes an infinite jump the first derivative of the wave function is discontinuous, but the wave function itself is still continuous.

To obtain the eigenfunctions $\phi_E(x)$ we can consider the different regions of constant potential separately and patch the solutions together. Thus, we start out by determining the solutions of the time-independent Schrödinger equation in constant potentials.

7.3.2 The free particle

The free particle is a particle moving without the influence of an external potential, that is, $V(x) = 0$. However, in quantum (as well as in classical) physics, the zero point of the energy is arbitrary. Thus, the free particle is equivalent to a particle moving under the influence of a constant potential $V(x) = V_0$, with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0, \tag{7.32}$$

with $V_0 \in \mathbb{R}$. The eigenvalue equation for the Hamiltonian (7.32), given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_E(x) = (E - V_0)\phi_E(x), \tag{7.33}$$

is formally solved by functions of the form

$$\phi_E(x) = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx}, \tag{7.34}$$

with the *wave number*

$$k = \frac{\sqrt{2m(E - V_0)}}{\hbar}, \tag{7.35}$$

for arbitrary values of $E \in \mathbb{R}$. However, the functions (7.34) diverge at $x \to \pm\infty$ for negative values of $E - V_0$. For the free particle on the whole real axis, we cannot interpret them in any meaningful way, and thus deduce that the eigenvalues of $\hat{H}$ are given by all real numbers $E \geq V_0$.

Even the eigenfunctions corresponding to these energies, however, are not square integrable, and can thus not be interpreted in the usual way as a probability amplitude to find a particle somewhere at a given time. They are however, a basis for all physically more meaningful wave functions in L^2.

Remark 37. We can interpret a wave function of the form

$$\psi_{\pm}(x) \propto \mathrm{e}^{\pm \mathrm{i}xk}, \tag{7.36}$$

a so-called *plane wave*, as a constant probability beam travelling from minus to plus infinity or plus to minus infinity, respectively. These wave functions are the extreme cases of Heisenberg's uncertainty principle, with accurately defined momentum, and totally unspecified position (describing a "completely *delocalised* particle"). Their probability flux is given by

$$j = \frac{\hbar}{2m\mathrm{i}} \left(\psi^* \psi' - \psi'^* \psi\right) = \pm \frac{\hbar k}{m}. \tag{7.37}$$

They are eigenfunctions of the momentum operator with eigenvalues $p = \hbar k$. Thus, they can be viewed as a stream of particles moving with constant velocity $\frac{p}{m}$.

Remark 38. The plane waves (7.36) fulfil the generalised orthonormality condition

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx} \mathrm{e}^{\mathrm{i}k'x} \mathrm{d}x = \delta(k - k'). \tag{7.38}$$

Remark 39. If we have a piecewise constant potential then in the separate regions that do not extend to infinity on both sides also the solutions (7.34) with energies $E < V_0$ are meaningful. They are more commonly expressed in the form

$$\phi_E(x) = C\mathrm{e}^{\kappa x} + D\mathrm{e}^{-\kappa x}, \tag{7.39}$$

with

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{7.40}$$

For regions that extend to $x_+\infty$ we need $C = 0$ and for regions that extend to $x \to -\infty$ it holds $D = 0$.

7.3.3 The infinite square well potential ("Particle in a box")

Let us now finally derive the eigenfunctions of a particle in an *infinite square well* (or "box") potential

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ \infty, & \text{otherwise,} \end{cases} \tag{7.41}$$

that we have already used numerous times. This system is an extreme case of a piecewise constant potential, where the potential is zero in a region $x \in [0, L]$ (the interior of the *box*) and infinite outside this region. Thus, outside the box the wave function has to be identical to zero. Inside the box, that is for $0 \leq x \leq L$, we have the solutions

$$\phi(x) = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx}, \tag{7.42}$$

with $k = \frac{\sqrt{2mE}}{\hbar}$. We know, however, that the wave function is continuous, and thus has to fulfil the boundary conditions

$$\phi(0) = 0 = \phi(L). \tag{7.43}$$

This yields the conditions

$$A + B = 0 \tag{7.44}$$
$$A\mathrm{e}^{\mathrm{i}kL} + B\mathrm{e}^{-\mathrm{i}kL} = 0 \tag{7.45}$$

for A and B. Inserting $B = -A$ into (7.45) yields

$$2\mathrm{i}A\sin(kL) = 0. \tag{7.46}$$

The choice $A = 0$ leads to a wave function that vanishes everywhere. The only physical meaningful wave functions exist for $\sin(kL) = 0$, which means

$$\frac{\sqrt{2mE}}{\hbar}L = n\pi, \tag{7.47}$$

for integer values of n, which yields the quantised energies

$$E_n = \frac{\pi^2\hbar^2}{2mL^2}\,n^2. \tag{7.48}$$

The corresponding eigenfunctions are given by

$$\phi_n(x) = 2\mathrm{i}A\sin\left(\frac{\sqrt{2mE_n}}{\hbar}\,x\right) = 2\mathrm{i}A\sin\left(\frac{\pi nx}{L}\right). \tag{7.49}$$

We can now choose A such that the $\phi_n(x)$ are normalised and real valued. The norm of $\phi_n(x)$ in dependence on A is given by

$$\begin{aligned}\int_0^L |\phi_n(x)|^2 &= 4|A|^2\int_0^L \sin^2\left(\frac{\pi nx}{L}\right)\mathrm{d}x \\ &= 2|A|^2\int_0^L \left(1-\cos\left(\frac{2\pi nx}{L}\right)\right)\mathrm{d}x \\ &= 2|A|^2L.\end{aligned} \tag{7.50}$$

Thus, the choice $A = \frac{-\mathrm{i}}{\sqrt{2L}}$ yields the normalised and real-valued wave functions

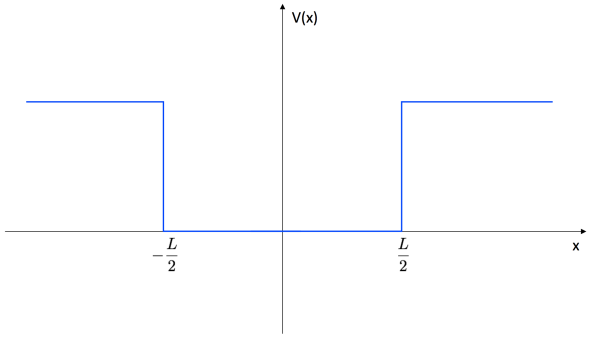
$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), & 0 \le x \le L \\ 0, \quad \text{otherwise,} \end{cases} \tag{7.51}$$

as given earlier without derivation in equation (2.25).

7.3.4 The finite square well potential ("Particle in a finite box")

The *finite square well potential* is similar to the previously considered infinite one, with the difference that the potential outside the central region is non-zero but finite. It is convenient to consider a symmetric version

$$V(x) = \begin{cases} 0, & |x| \le \frac{L}{2} \\ V_0, & \text{otherwise.} \end{cases} \tag{7.52}$$



The solutions of the time-independent Schrödinger equation in the separate regions are of the form $a\mathrm{e}^{\mathrm{i}kx} + b\mathrm{e}^{-\mathrm{i}kx}$ with $k = \sqrt{2m(E - V_j)}/\hbar$, where

V_j is the value of the constant potential in region j. For values $E > V_j$, $k \in \mathbb{R}$ this can be equivalently written as $\tilde{a}\cos(kx) + \tilde{b}\sin(kx)$, while for $E < V_j$ we have $\kappa = \sqrt{2m(V_j - E)}/\hbar \in \mathbb{R}$, and the solutions take the form $a\mathrm{e}^{-\kappa x} + b\mathrm{e}^{\kappa x}$. That is we make the ansatz

$$\phi_E(x) = \begin{cases} C_1\mathrm{e}^{\kappa x} + C_2\mathrm{e}^{-\kappa x}, & x \leq -L/2 \\ A\cos(kx) + B\sin(kx), & -L/2 < x \leq L/2 \\ D_1\mathrm{e}^{\kappa x} + D_2\mathrm{e}^{-\kappa x}, & x > L/2, \end{cases} \tag{7.53}$$

with $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$ for the solution of the time-independent Schrödinger equation.

Here we are looking for *bound states*, that is $\phi(x \to \pm\infty) \to 0$. From the general solution (7.53) we deduce that this is only possible for $E < V_0$, and that further we need $C_2 = 0 = D_1$. Thus, the solutions are of the form

$$\phi_E(x) = \begin{cases} C\mathrm{e}^{\kappa x}, & x \leq -L/2 \\ A\cos(kx) + B\sin(kx), & -L/2 < x \leq L/2 \\ D\mathrm{e}^{-\kappa x}, & x > L/2. \end{cases} \tag{7.54}$$

The wave function $\phi_E(x)$ and its first derivative with respect to x have to be continuous everywhere. This is automatically fulfilled in the separate regions, but it imposes four boundary conditions between the different regions.

Exercise 12. Find the four boundary conditions the eigenfunctions need to fulfil. Use the fact that the symmetry of the potential means that the eigenfunctions are either even or odd eigenfunction, and verify that even eigenfunctions have to fulfil the conditions

$$C\mathrm{e}^{-\kappa L/2} = A\cos(kL/2) \tag{7.55}$$

$$\kappa C\mathrm{e}^{-\kappa L/2} = kA\sin(kL/2), \tag{7.56}$$

and odd eigenfunctions have to fulfil the conditions

$$C\mathrm{e}^{-\kappa L/2} = -B\sin(kL/2) \tag{7.57}$$

$$\kappa C\mathrm{e}^{-\kappa L/2} = kB\cos(kL/2). \tag{7.58}$$

These conditions can only be fulfilled simultaneously for specific values of the energy E, leading to the quantisation conditions

$$\kappa = k\tan(kL/2) \tag{7.59}$$

and

$$\kappa = -k\cot(kL/2), \tag{7.60}$$

for even and odd eigenfunctions, respectively. We can rewrite these in terms of the energy using the identities

$$\begin{aligned} \kappa/k &= \sqrt{\frac{2mV_0}{\hbar^2k^2} - 1} \\ k &= \sqrt{2mE}/\hbar, \end{aligned} \tag{7.61}$$

to find

$$\tan\left(\frac{\sqrt{2mE}L}{2\hbar}\right) = \sqrt{\frac{V_0}{E} - 1}\,, \tag{7.62}$$

and

$$-\cot\left(\frac{\sqrt{2mE}L}{2\hbar}\right) = \sqrt{\frac{V_0}{E} - 1}\,, \tag{7.63}$$

for even and odd eigenfunctions, respectively.

These conditions have to be solved numerically or graphically to find the quantised energies. We will discuss this further in the lecture.

Chapter 8

Quantum dynamics

In this chapter we shall turn away from the spectral problems, and focus our attention on the dynamical features of quantum theory. The most interesting features of observable things are often those that change in time, after all. We shall discuss dynamics of expectation values, which yields a version of the famous *Heisenberg equations* of motion, which can be viewed as an alternative to Schrödinger's dynamical equation in quantum mechanics. We then turn to the discussion of quantum dynamics from a Lie algebraic perspective, and finish with an example of *dynamical tunneling*.

8.1 Dynamics of expectation values

From the time-dependent Schrödinger equation, $\mathrm{i}\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle$, we can deduce a dynamical equation for observable expectation values $\langle\hat{A}\rangle$: We have by definition

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{8.1}$$

Thus, we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle = \frac{\langle\dot{\psi}|\hat{A}|\psi\rangle + \langle\psi|\dot{\hat{A}}|\psi\rangle + \langle\psi|\hat{A}|\dot{\psi}\rangle}{\langle\psi|\psi\rangle} - \frac{\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle^2}\langle\psi|\hat{A}|\psi\rangle. \tag{8.2}$$

From the Schrödinger equation we know

$$|\dot{\psi}\rangle = -\frac{\mathrm{i}}{\hbar}\hat{H}|\psi\rangle, \quad \text{and} \quad \langle\dot{\psi}| = \frac{\mathrm{i}}{\hbar}\langle\psi|\hat{H}, \tag{8.3}$$

thus, the overall norm is conserved, $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\psi\rangle = 0$ and we find

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle &= \frac{\frac{\mathrm{i}}{\hbar}\langle\psi|\hat{H}\hat{A}|\psi\rangle + \langle\psi|\dot{\hat{A}}|\psi\rangle - \frac{\mathrm{i}}{\hbar}\langle\psi|\hat{A}\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{\mathrm{i}}{\hbar}\langle\hat{H}\hat{A} - \hat{A}\hat{H}\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle.\end{aligned} \tag{8.4}$$

Or, using the commutator,

$$\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\langle[\hat{H},\hat{A}]\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle. \tag{8.5}$$

This is one formulation of the famous *Heisenberg equation* of motion for observables, which can be used as the foundational dynamical equation of quantum mechanics, as an alternative of Schrödinger's equation. Comparing the Heisenberg equation to the classical equation of motion (1.16) for a phase space variable $A(p,q)$ we observe a striking similarity if we associate expectation values with classical variables and interpret the commutator, or more precisely $\mathrm{i}/\hbar$ times the commutator, as a *quantum Poisson bracket*.

The Ehrenfest theorem

The special case of the equations of motion for the expectation values of position and momentum for a system with Hamiltonian of the type

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{q}) \tag{8.6}$$

forms the basis of what is referred to as the *Ehrenfest theorem*, which we shall consider in what follows. From equation (8.5) and the form of the Hamiltonian (8.6) we find

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle &= \frac{\mathrm{i}}{\hbar}\langle[\frac{\hat{p}^2}{2m}, \hat{q}]\rangle \\ &= \frac{\mathrm{i}}{2\hbar m}\langle[\hat{p}^2, \hat{q}]\rangle \\ &= \frac{\mathrm{i}}{2\hbar m}\langle\hat{p}[\hat{p}, \hat{q}] + [\hat{p}, \hat{q}]\hat{p}\rangle. \end{aligned} \tag{8.7}$$

Recalling the commutation relation between position and momentum operator, $[\hat{q}, \hat{p}] = \mathrm{i}\hbar$, this reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle = \frac{\langle\hat{p}\rangle}{m}. \tag{8.8}$$

For the momentum operator we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = \frac{\mathrm{i}}{\hbar}\langle[\hat{V}(\hat{q}), \hat{p}]\rangle. \tag{8.9}$$

To calculate the commutator between the momentum operator and the potential, it is convenient to use the position representation, in which we have

$$[\hat{V}(\hat{q}), \hat{p}] = -\mathrm{i}\hbar[V(x), \frac{\partial}{\partial x}], \tag{8.10}$$

applied to a test function $\psi(x)$,

$$\begin{aligned} -\mathrm{i}\hbar\,[V(x), \frac{\partial}{\partial x}]\,\psi(x) &= -\mathrm{i}\hbar V(x)\psi'(x) + \mathrm{i}\hbar\frac{\partial}{\partial x}(V(x)\psi(x)) \\ &= -\mathrm{i}\hbar V(x)\psi'(x) + \mathrm{i}\hbar V'(x)\psi(x) + \mathrm{i}\hbar V(x)\psi'(x) \\ &= \mathrm{i}\hbar V'(x)\psi(x) \end{aligned} \tag{8.11}$$

Translating this back to the abstract operator notation this is

$$[\hat{V}(\hat{q}), \hat{p}] = \mathrm{i}\hbar\frac{\mathrm{d}V(\hat{q})}{\mathrm{d}\hat{q}}, \tag{8.12}$$

and thus we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = -\langle\frac{\partial\hat{V}}{\partial\hat{q}}\rangle. \tag{8.13}$$

In summary we have obtained the set of equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle = \frac{\langle\hat{p}\rangle}{m}, \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = -\langle\frac{\partial\hat{V}}{\partial\hat{q}}\rangle, \tag{8.14}$$

which are strikingly similar in form to the classical equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}q = \frac{p}{m}, \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}p = -\frac{\partial V}{\partial q}, \tag{8.15}$$

a fact that is often referred to as the *Ehrenfest theorem*.

Notwithstanding the formal similarity, there are of course important differences between quantum and classical dynamics. On the level of the Ehrenfest theorem, this is due to the fact that in general

$$\langle \frac{\partial \hat{V}}{\partial \hat{q}} \rangle \neq \frac{\partial V(\langle \hat{q} \rangle)}{\partial \langle \hat{q} \rangle}. \tag{8.16}$$

Consider for example the case $\hat{V}(\hat{q}) = \hat{q}^4$. Here we have

$$\frac{\partial \hat{V}(\langle \hat{q} \rangle}{\partial \langle \hat{q} \rangle} = 4\langle \hat{q} \rangle^3, \tag{8.17}$$

while

$$\langle \frac{\partial \hat{V}}{\partial \hat{q}} \rangle = 4\langle \hat{q}^3 \rangle. \tag{8.18}$$

The two expressions in equation (8.16) are, however, similar for potentials that are polynomials of $\hat{q}$ of order two or lower. For more general potentials equations (8.14) in fact do not even form a closed set of equations (as the left side of the time derivative of $\langle \hat{p} \rangle$ is not only a function of $\langle \hat{q} \rangle$ and $\langle \hat{p} \rangle$).

Literary Excursion

In the following I provide a translation of a short excerpt from the novel *Dirac* by Dietmar Dath (Surkamp 2006) to provide some further insight into the development of quantum mechanics, albeit in the form of a literary supplement.

Just like a melody, which the whistling lips are faster to grasp than the conscious mind, Heisenberg's mathematics returns to the focus of Dirac's attention. Non-commutativity, this times that is different from that times this. A pale-blue bird thrusts itself onto the strong wind just above Dirac's head, struggling, staggering, spinning, re-balancing, it positions itself tangentially to the air stream, and then rises again, very fast and very high. Dirac is viewing the bird in a coordinate plane, seeing it rotating, and fleeing upwards.

Position and velocity, where the bird is thrown towards, and how it is flapping its wings: Sky and puddle, wind and water, bird and – fish? "Poisson", Dirac says.

That's it! Poisson brackets. Siméon Denis Poisson, seventeen hundred eighty one to eighteen hundred forty. Non-commutativity... Where has he read about this? What was it? There seems to be a connection. Or is he just grasping at straws? Heisenberg's commutator: $uv - vu$, and the relation between the two quantities in this formalism for phase-space transforms. ...This is only the faintest memory: Old mathematics, which might come to rescue Heisenberg's new physics. Dirac is leaping over the road-side ditch without a thought on what he is doing, and he is now walking right across the muddy meadow. Every step slurping, Dirac is in a hurry: He has to go home, has to look it up, find out what's going on there... Poisson, non-commutativity – everything.

Dirt splashing on his trousers, his joints cracking, he is hurrying on. It can't be true. The similarity of these two forms must be a coincidence, just like a rhyme in a poem or a harmony of two voices. It would be too strange for such a coincidence to actually mean anything. Already he has a feeling that this thought, which had only just occurred to him, might be implausible, but his excitement is growing at the same time: What if there was something to it? After a few hundred metres of cross-country tracking he is now reaching a footpath and finding himself panting for air, staggering, dizzy: He had been running. He has left the rural area behind and is now in the town. He is pushed forward into his thoughts by a tailwind, which is seizing him just as it had seized the bird before him.

Finally he reaches his door, hectically searching his coat pocket for his key. As he tries to unlock the door too fast, the key gets stuck. He is swearing under his breath. He has to get in there, look it up, clear definitions, order! He is rattling at the lock, which finally releases the key. Dirac immediately reinserts it and this time the door opens. Without even taking off his coat Dirac is

rushing through his room, searching his books, his lecture notes, kneeling on the floor, opening all the drawers.

The storm that had been raging outside earlier is revived again in this room; pages are flying, eyes are searching, but nothing: canonical transformations, linear mappings, differential equations, textbooks, mathematical tables. All of this is much too fundamental. Nothing on Poisson brackets, no hint. But he did see it. Did read it: In a book, not in a lecture note.

Finally he is sitting in the midst of the chaos he has produced, panting. He takes off his coat and it makes him chuckle: Sunday night. All libraries closed. He runs his fingers through his hair, as if what he is looking for might be stuck in there.

Dreadful, euphoric night: Dirac's heart is pounding in his throat, half asleep he is imagining himself as a little bird in the wind, throwing himself from left to right. If it really was possible to express things this way, if one could formulate a type of Hamiltonian dynamics using non-commutative Poisson-brackets... If that was the key...

Dawn is breaking. Dirac gets up. His joints are painful. He is extraordinarily weary, as after hard labour. After a quick superficial wash he gets dressed and leaves the house, walking straight towards the faculty library. He is the first one there. The librarian allows him in, shaking his head. Dirac is rushing past long rows of bookshelves, he knows his way around here.

He takes a left turn at the big cross-bar window in front of one of the columns. There, at breast height, is Whittaker's "Analytical Dynamics". Dirac quickly finds what he was looking for. The letters are flickering, and he is finding it difficult to read. Yet, his intuition had not failed him. He now has his own key to the latest physics...

8.2 Lie groups and Lie algebras in quantum dynamics

8.2.1 A quick overview

The time evolution in quantum mechanics is closely related to the concept of (Lie) groups. In this section, I will give a brief summary of the most important concepts in this context.

We begin with a brief reminder of the concept of a

Group. A *group* is a set $\mathcal{G}$ of elements, together with a map $\circ : \mathcal{G} \times \mathcal{G} \to \mathcal{G}$, which fulfil the following three properties:

- The map is associative, i.e. $(a \circ b) \circ c = a \circ (b \circ c)$, for all $a, b, c \in \mathcal{G}$,
- The group contains an identity element e with $e \circ a = a \circ e = a$ for all $a \in \mathcal{G}$,
- Every element has an inverse element in the group, often denoted by a^{-1}, such that $a \circ a^{-1} = a^{-1} \circ a = e$.

A *representation* of a group can be thought of as a realisation of group elements as linear operators on a linear vector space $\mathcal{V}$, that is, a map (*a group homomorphism*) $g \to \hat{D}(g)$, from $\mathcal{G}$ to $GL(\mathcal{V})$ (the group formed by the invertible linear maps on the vector space $\mathcal{V}$), which fulfils

$$\hat{D}(g_1 \circ g_2) = \hat{D}(g_1)\hat{D}(g_2). \tag{8.19}$$

Thus we have $\hat{D}(g^{-1}) = (\hat{D}(g))^{-1}$, and $\hat{D}(e) = \hat{I}$, where $\hat{I}$ denotes the identity on $\mathcal{V}$. A representation is *faithful* if the map $g \to \hat{D}(g)$ is injective.

A *continuous group* is a group with elements that continuously depend on parameters, i.e. the group elements are functions of a set of parameters. The set of unitary operations on a Hilbert space together with the consecutive application of unitary operations as the group map, form a continuous group.

A special type of continuous groups are *Lie groups*. Whole lectures and textbooks are devoted to the topic of Lie groups. We will only devote a couple of paragraphs, sacrificing rigour for an intuitive idea. Broadly speaking, an n-dimensional *Lie group* is a continuous group, the elements g

of which can be represented as C^n functions of n real parameters, with $g(0) = e$. Thus, Lie groups are both groups and analytical manifolds.

If $\hat{D}(g)$ is a representation of a Lie group element, we write for short $\hat{D}(x) = \hat{D}(g(x))$, and $\hat{D}(0) = \hat{I}$. Since a Lie group element is a differentiable function of the parameters, for small values of x we can expand an element into a power series with the first two terms

$$\hat{D}(x) = \hat{I} + \mathrm{i}\sum_{j=1}^{n} x_j \hat{T}_j + \ldots, \tag{8.20}$$

with

$$\hat{T}_j = -\mathrm{i}\left.\frac{\partial \hat{D}}{\partial x_j}\right|_{x=0}. \tag{8.21}$$

Remark 40. The factor of i in (8.20) and (8.21) is common in physics, but is not usually used in the mathematics literature.

Remark 41. The higher order terms in (8.20) are in general complicated.

The operators $\hat{T}_j$ in (8.21) are called the *generators* of the group. Let us for simplicity consider a one-dimensional group with representation $\hat{D}(x)$ with $x \in \mathbb{R}$. When the generator $\hat{T}$ is known the group structure allows to represent group elements not only for small but for arbitrary x, since $\hat{D}(2\Delta x) = \hat{D}(\Delta x)\hat{D}(\Delta x) = (\hat{D}(\Delta x))^2$ and $\hat{D}(m\Delta x) = (\hat{D}(\Delta x))^m$, and thus, if we define $x = m\Delta x$ we have

$$\hat{D}(x) = (\hat{D}(\Delta x))^m \approx (1 + \mathrm{i}\Delta x\hat{T})^m = (1 + \mathrm{i}\frac{x}{m}\hat{T})^m \xrightarrow[m\to\infty]{} \mathrm{e}^{\mathrm{i}x\hat{T}}. \tag{8.22}$$

Remark 42. Here the similarity to the relation between our time-evolution operator and our Hamiltonian for time-independent systems should become apparent.

The n generators of an n dimensional Lie group form a *Lie algebra*. A *Lie algebra* is a vector space G with a map $[\cdot,\cdot] : G \times G \to G$, a so-called *Lie bracket*, that maps each ordered pair of algebra elements to a third algebra element, and that is anti-symmetric, bilinear, and fulfils the Jacobi identity $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$ (just like our Poisson brackets and commutators).

A simple example of a finite Lie algebra we encounter in quantum mechanics consists of the position and the momentum operators and the identity, since we have

$$[\hat{q},\hat{p}] = \mathrm{i}\hbar\hat{I}. \tag{8.23}$$

This algebra corresponds to the group of translations in phase space.

Another example is the algebra associated to the harmonic oscillator, spanned by the identity, $\hat{a}$, $\hat{a}^\dagger$, and $\hat{N}$, with

$$[\hat{a},\hat{a}^\dagger] = \hat{I}, \quad [\hat{N},\hat{a}] = -\hat{a}, \quad [\hat{N},\hat{a}^\dagger] = \hat{a}^\dagger. \tag{8.24}$$

The corresponding group consists of translations and rotations in phase space.

An important consequence for quantum mechanics is that if a Hamiltonian is an element of a Lie algebra, that is, a linear combination of the Lie algebra elements, $\hat{K}_j$,

$$\hat{H} = \sum_j c_j \hat{K}_j, \tag{8.25}$$

then the corresponding time evolution operator can be expressed as

$$\hat{U} = \mathrm{e}^{\mathrm{i}\sum_j \alpha_j \hat{K}_j}, \tag{8.26}$$

in what is called the *Magnus* form, or alternatively as

$$\hat{U} = \prod_j \mathrm{e}^{\mathrm{i}\beta_j \hat{K}_j}, \tag{8.27}$$

in the so-called *Wei Norman* form. Importantly this still holds if the coefficients c_j in the Hamiltonian are time dependent.

When considering the time evolution of expectation values (in the Heisenberg equation), we encounter expressions of the form $\hat{U}^\dagger \hat{A} \hat{U}$. Explicitly evaluating these can be challenging unless the Hamiltonian and the observable $\hat{A}$ are elements of a nice Lie algebra. In general we have

Theorem 9 (Hadamard lemma)**.**

$$\mathrm{e}^{s\hat{X}}\hat{Y}\mathrm{e}^{-s\hat{X}} = \hat{Y} + s[\hat{X},\hat{Y}] + \frac{s^2}{2!}[\hat{X},[\hat{X},\hat{Y}]] + \frac{s^3}{3!}[\hat{X},[\hat{X},[\hat{X},\hat{Y}]]] + ..., \tag{8.28}$$

where $\hat{X}$ and $\hat{Y}$ are linear operators and $s \in \mathbb{C}$ is a complex constant.

Proof. We consider $f(s) := \mathrm{e}^{s\hat{X}}\hat{Y}\mathrm{e}^{-s\hat{X}}$ as an operator valued function of the complex variable s, and Taylor expand around $s = 0$:

$$\hat{f}(s) = \sum_n \hat{f}^{(n)}(0)\frac{s^n}{n!}. \tag{8.29}$$

We have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}s}\mathrm{e}^{s\hat{X}}\hat{Y}\mathrm{e}^{-s\hat{X}} &= \mathrm{e}^{s\hat{X}}\hat{X}\hat{Y}\mathrm{e}^{-s\hat{X}} - \mathrm{e}^{s\hat{X}}\hat{Y}\hat{X}\mathrm{e}^{-s\hat{X}} \\ &= \mathrm{e}^{s\hat{X}}[\hat{X},\hat{Y}]\mathrm{e}^{-s\hat{X}}, \end{aligned} \tag{8.30}$$

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}s^2}\mathrm{e}^{s\hat{X}}\hat{Y}\mathrm{e}^{-s\hat{X}} &= \mathrm{e}^{s\hat{X}}\hat{X}[\hat{X},\hat{Y}]\mathrm{e}^{-s\hat{X}} - \mathrm{e}^{s\hat{X}}[\hat{X},\hat{Y}]\hat{X}\mathrm{e}^{-s\hat{X}} \\ &= \mathrm{e}^{s\hat{X}}[\hat{X},[\hat{X},\hat{Y}]]\mathrm{e}^{-s\hat{X}}, \end{aligned} \tag{8.31}$$

and so forth. Inserting this into the Taylor expansion yields equation (8.28). □

Exercise 13. Use the Hadamard lemma and the fundamental commutator to show that

$$\mathrm{e}^{\mathrm{i}a\hat{p}_1/\hbar}\hat{q}_1\mathrm{e}^{-\mathrm{i}a\hat{p}_1/\hbar} = \hat{q}_1 + a. \tag{8.32}$$

8.2.2 Reminder: The group $SU(2)$

A group that is of great importance in the theory of angular momentum, which we will discuss in the next Chapter, is the group $SU(2)$. The corresponding Lie algebra $su(2)$ can be spanned by three elements $\hat{J}_k$, with $k = 1, 2, 3$ that fulfill the commutation relations

$$[\hat{J}_j, \hat{J}_k] = \mathrm{i}\hbar\sum_l \epsilon_{jkl}\hat{J}_l, \tag{8.33}$$

where

$$\epsilon_{jkl} = \begin{cases} 1, & j,k,l \text{ cyclic} \\ -1, & j,k,l \text{ anticyclic} \\ 0, & \text{otherwise,} \end{cases} \tag{8.34}$$

is the *Levi-Civita symbol.*

You have probably encountered the group $SU(2)$ before, as the group of complex unitary 2×2 matrices with determinant one, i.e. the set of matrices

$$SU(2) = \{S \in \mathbb{C}^{2\times 2} | S^\dagger = S^{-1} \text{ and } \det S = 1\}, \tag{8.35}$$

which is a Lie group under matrix multiplication.

In the mathematics literature, the associate Lie algebra is commonly defined as the set of matrices generating the group elements via the exponential map, which in the case of $SU(2)$ consists of complex anti-Hermitian 2×2 matrices with trace zero. In the physics literature we tend to include

a factor of i into the exponent in the exponential map resulting in the algebra of complex Hermitian 2×2 matrices with trace 1. A basis for these is given by the matrices

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8.36}$$

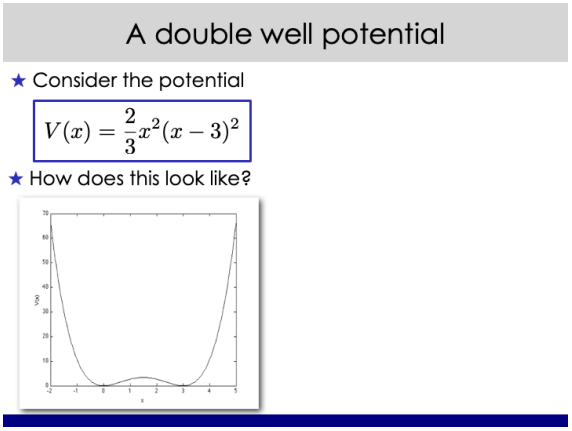
These matrices are also known as the *Pauli matrices*. They fulfil the commutation relations

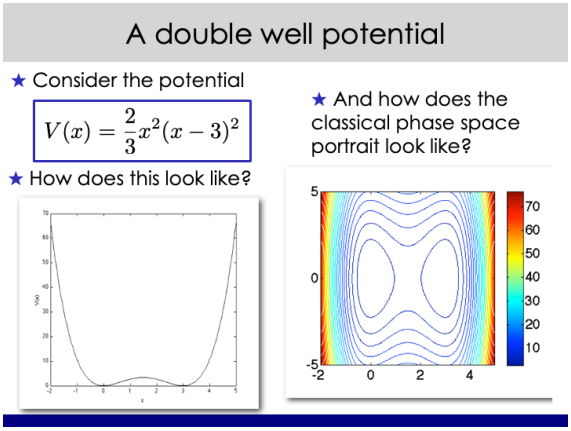
$$[\hat{\sigma}_j, \hat{\sigma}_k] = 2\mathrm{i} \sum_l \epsilon_{jkl} \hat{\sigma}_l. \tag{8.37}$$

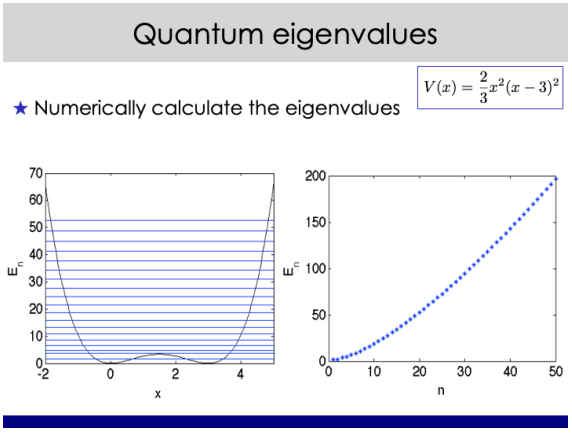
$SU(2)$ is commonly associated with complex 2×2 matrices. However, it has higher dimensional representations which will be related to quantum mechanical angular momentum, as we shall see in Chapter 9.

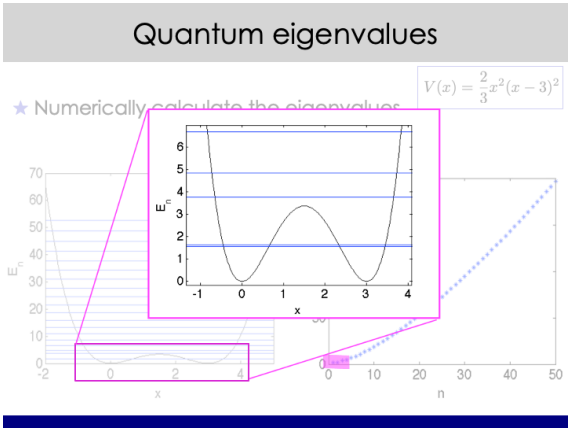
8.3 Dynamical Tunneling

I include the slides from the video on dynamical tunneling here.









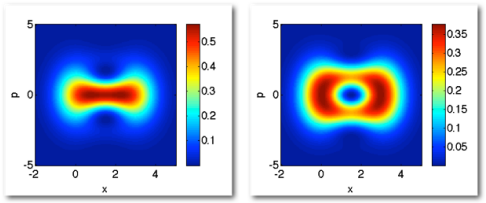
Phase-space picture of eigenfunctions

★ Husimi representation of two lowest energy eigenstates (Overlap with coherent states)

$$\rho_\psi(p,q) = \frac{1}{2\pi\hbar}|\langle z|\psi\rangle|^2$$

$$|z\rangle = \mathrm{e}^{-\frac{|z|^2}{2}} \sum_n \frac{z^n}{\sqrt{n!}}|n\rangle$$

$$z = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}\,q + \frac{1}{\sqrt{m\omega}}p\right)$$



Tunneling

★ What might happen to an initial Gaussian wave packet centred at the left minimum (x=0) with momentum zero?

★ And what does that have to do with the two lowest eigenfunctions?

Tunneling

★ What might happen to an initial Gaussian wave packet centred at the left minimum (x=0) with momentum zero?

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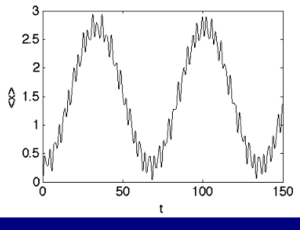
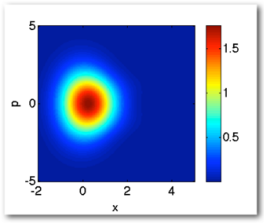


Tunneling

★ Husimi function of an equal superposition of the two lowest states

$$\psi(x,t=0) = \tfrac{1}{\sqrt{2}}(\phi_1(x) + \phi_2(x))$$



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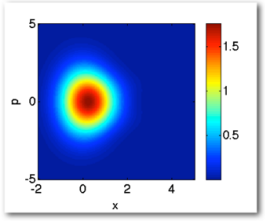


★ How does this evolve in time?

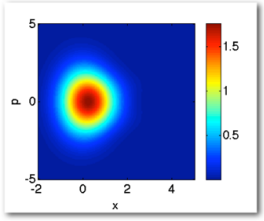
★ Oscillation with period

$$T = \frac{2\pi}{E_2 - E_1}$$

Tunneling

★ Husimi function of an equal superposition of the two lowest states

$$\psi(x,t=0) = \tfrac{1}{\sqrt{2}}(\phi_1(x) + \phi_2(x))$$



★ How does this evolve in time?

★ Oscillation with period

$$T = \frac{2\pi}{E_2 - E_1}$$

★ From numerical results:

$$E_2 - E_1 = 0.093 \;\Rightarrow T = 67.6$$

Chapter 9

Angular momentum

9.1 Definition of angular momentum - classical and quantum

In this chapter we move beyond one-dimensional systems and consider angular momentum. In classical mechanics the angular momentum of a particle moving in three spatial dimensions with spatial coordinate $\vec{q} \in \mathbb{R}^3$ and momentum $\vec{p} \in \mathbb{R}^3$ is given by

$$\vec{L} = \vec{q} \times \vec{p}, \tag{9.1}$$

or in components

$$L_1 = q_2 p_3 - q_3 p_2, \quad L_2 = q_3 p_1 - q_1 p_3, \quad \text{and} \quad L_3 = q_1 p_2 - q_2 p_1. \tag{9.2}$$

In quantum mechanics, we can as well consider a particle in three dimensional space $\mathbb{R}^3$, with position and momentum operators $\hat{q} = (\hat{q}_1, \hat{q}_2, \hat{q}_3)^T$, and $\hat{p} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)^T$, whose components fulfil the canonical commutation relations

$$[\hat{q}_j, \hat{p}_k] = \mathrm{i}\hbar\delta_{jk}, \qquad [\hat{q}_j, \hat{q}_k] = 0 = [\hat{p}_j, \hat{p}_k]. \tag{9.3}$$

In analogy to classical mechanics we can then define an operator associated to the *orbital angular momentum* as

$$\hat{L} = \hat{q} \times \hat{p}, \tag{9.4}$$

that is, an operator with the three components

$$\begin{aligned} \hat{L}_1 &= \hat{q}_2\hat{p}_3 - \hat{q}_3\hat{p}_2 \\ \hat{L}_2 &= \hat{q}_3\hat{p}_1 - \hat{q}_1\hat{p}_3 \\ \hat{L}_3 &= \hat{q}_1\hat{p}_2 - \hat{q}_2\hat{p}_1. \end{aligned} \tag{9.5}$$

The components of the orbital angular momentum fulfil the commutation relations

$$[\hat{L}_1, \hat{L}_2] = \mathrm{i}\hbar\hat{L}_3, \quad [\hat{L}_2, \hat{L}_3] = \mathrm{i}\hbar\hat{L}_1, \quad [\hat{L}_3, \hat{L}_1] = \mathrm{i}\hbar\hat{L}_2, \tag{9.6}$$

which are just the commutation relations of the $su(2)$ algebra, written more compactly as

$$[\hat{L}_j, \hat{L}_k] = \mathrm{i}\hbar \sum_l \epsilon_{jkl}\hat{L}_l. \tag{9.7}$$

In quantum mechanics, we make the following definition:

Quantum angular momentum An operator with three Hermitian operator components $\hat{J}_{1,2,3}$ fulfilling the commutation relations

$$[\hat{J}_j, \hat{J}_k] = \mathrm{i}\hbar \sum_l \epsilon_{jkl}\hat{J}_l, \tag{9.8}$$

is an *angular momentum operator*.

The total angular momentum operator is then defined as

$$\hat{J}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2. \tag{9.9}$$

It can be easily verified that $[\hat{J}^2, \hat{J}_j] = 0$.

Remark 43. In the following we shall use the letter J to denote generic quantum angular momentum, while we reserve the letter L to denote orbital angular momentum, which can be defined as (9.5) in some given coordinate system.

9.2 Angular momentum and rotations

The above definition of angular momentum relates it to the group $SU(2)$, which, is a *double cover* of the group $SO(3)$, which can be represented as rotations in $\mathbb{R}^3$. Intuitively it makes perfect sense, that angular momentum is thus related to rotations. Technically speaking, the angular momentum operators are the generators of infinitesimal rotations. Here we shall investigate an intuitive connection between angular momentum and rotations, by showing that the time-evolution where the angular momentum operators act as Hamiltonians, are rotations of the coordinate system.

9.2.1 Reminder: Rotations in $\mathbb{R}^3$

The rotations in $\mathbb{R}^3$ are a non-commutative group. A rotation in $\mathbb{R}^3$ can be described by three parameters: the direction of the axis of rotation (two parameters) and the angle of rotation, and can be expressed by an orthogonal (real unitary) 3×3 matrix. There are three fundamental rotations that can be used as a basis for all other rotations, the rotations around the x, y- and z-axes, whose matrices are given by:

$$R_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix}, \quad R_y(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi \\ 0 & 1 & 0 \\ -\sin\phi & 0 & \cos\phi \end{pmatrix},$$

and

$$R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Applying for example $R_x(\phi)$ to $\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ yields:

$$R_x(\phi) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y\cos\phi - z\sin\phi \\ y\sin\phi + z\cos\phi \end{pmatrix},$$

i.e. a rotation around the x-axis by the angle ϕ.

9.2.2 Action of the $e^{i\phi\hat{L}_j/\hbar}$ on the position operators

Consider a quantum system in $\mathbb{R}^3$ described by the state $|\psi\rangle$. We shall now show that the time evolution with a Hamiltonian $\hat{H} = \hat{L}_j$ (orbital angular momentum) corresponds to a rotation of the coordinate system. The time-evolved state is given by $|\psi(t)\rangle = e^{-i\hat{L}_j t/\hbar}|\psi(0)\rangle$. Thus, the expectation value of an observable $\hat{A}$ at time t is given by

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(0)|e^{i\hat{L}_j t/\hbar}\hat{A}e^{-i\hat{L}_j t/\hbar}|\psi(0)\rangle. \tag{9.10}$$

Alternatively, we can interpret this as the expectation value of the operator $\mathrm{e}^{\mathrm{i}\hat{L}_j t/\hbar}\hat{A}\mathrm{e}^{-\mathrm{i}\hat{L}_j t/\hbar}$ in the state at time zero. Let us consider the expectation values of the position operators $\hat{q}_{1,2,3}$. Denote the expectation value of $\hat{q}$ at time zero by the vector $\vec{Q} = (Q_1, Q_2, Q_3)^T \in \mathbb{R}^3$.

To calculate $\mathrm{e}^{\mathrm{i}\hat{L}_j t/\hbar}\hat{q}_k\mathrm{e}^{-\mathrm{i}\hat{L}_j t/\hbar}$ we can use the Hadamard lemma 8.28. From the definition of the components of the orbital angular momentum (9.5) we find the commutators

$$[\hat{L}_j, \hat{q}_k] = i\hbar\epsilon_{jkl}\hat{q}_l. \tag{9.11}$$

Using these and the Hadamard lemma we can calculate the $\mathrm{e}^{i\phi\hat{L}_j/\hbar}\hat{q}_k\mathrm{e}^{-i\phi\hat{L}_j/\hbar}$. Let us consider the examples $\mathrm{e}^{i\phi\hat{L}_1/\hbar}\hat{q}_j\mathrm{e}^{-i\phi\hat{L}_1/\hbar}$. Since $[\hat{L}_j, \hat{q}_j] = 0$, we trivially have

$$\mathrm{e}^{i\phi\hat{L}_1/\hbar}\hat{q}_1\mathrm{e}^{-i\phi\hat{L}_1/\hbar} = \hat{q}_1. \tag{9.12}$$

To evaluate $\mathrm{e}^{i\phi\hat{L}_1/\hbar}\hat{q}_2\mathrm{e}^{-i\phi\hat{L}_1/\hbar}$ we need to calculate the nested commutators $[\hat{L}_1, [\hat{L}_1, [..., [\hat{L}_1, \hat{q}_2]...]]]$. This can be done iteratively, starting from $[\hat{L}_1, \hat{q}_2] = i\hbar\hat{q}_3$:

$$\begin{aligned}
[\hat{L}_1, [\hat{L}_1, \hat{q}_2]] &= i\hbar[\hat{L}_1, \hat{q}_3] = \hbar^2\hat{q}_2 \\
[\hat{L}_1, [\hat{L}_1, [\hat{L}_1, \hat{q}_2]]] &= \hbar^2[\hat{L}_1, \hat{q}_2] = i\hbar^3\hat{q}_3 \\
[\hat{L}_1, [\hat{L}_1, [\hat{L}_1, [\hat{L}_1, \hat{q}_2]]]] &= i\hbar^3[\hat{L}_1, \hat{q}_3] = \hbar^4\hat{q}_2 \\
&\vdots
\end{aligned}$$

Remembering the Taylor expansions of sin and cos:

$$\begin{aligned}
\sin(x) &= x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + ... \\
\cos(x) &= 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + ...
\end{aligned}$$

we realise that

$$\mathrm{e}^{i\phi\hat{L}_1/\hbar}\hat{q}_2\mathrm{e}^{-i\phi\hat{L}_1/\hbar} = \hat{q}_2\cos(\phi) - \hat{q}_3\sin(\phi).$$

Similarly we find

$$\mathrm{e}^{i\phi\hat{L}_1/\hbar}\hat{q}_3\mathrm{e}^{-i\phi\hat{L}_1/\hbar} = \hat{q}_3\cos(\phi) + \hat{q}_2\sin(\phi),$$

and so on. That is, we have

$$\vec{Q}(t) := \langle\psi(0)|\mathrm{e}^{\mathrm{i}\hat{L}_j t/\hbar}\hat{q}\mathrm{e}^{-\mathrm{i}\hat{L}_j t/\hbar}|\psi(0)\rangle = R_j(t)\vec{Q}, \tag{9.13}$$

where $R_j(t)$ is the rotation matrix around the axis j by an angle t, and $\vec{Q}$ is the vector of expectation values of the position operators at time zero.

9.2.3 Action of the $\mathrm{e}^{\mathrm{i}\phi\hat{J}_j/\hbar}$ on the angular momentum operators

Similarly to the considerations above we can use the Hadamard lemma to calculate $\mathrm{e}^{i\phi\hat{J}_j/\hbar}\hat{J}_k\mathrm{e}^{-i\phi\hat{J}_j/\hbar}$: Trivially we have

$$\mathrm{e}^{i\phi\hat{J}_j/\hbar}\hat{J}_j\mathrm{e}^{-i\phi\hat{J}_j/\hbar} = \hat{J}_j. \tag{9.14}$$

Let us now consider the example $\mathrm{e}^{i\phi\hat{J}_1/\hbar}\hat{J}_2\mathrm{e}^{-i\phi\hat{J}_1/\hbar}$. Again, we need to calculate the nested commutators $[\hat{J}_1, [\hat{J}_1, [..., [\hat{J}_1, \hat{J}_2]...]]]$. Similarly to above, this can be done iteratively, starting from $[\hat{J}_1, \hat{J}_2] = i\hbar\hat{J}_3$:

$$\begin{aligned}
[\hat{J}_1, [\hat{J}_1, \hat{J}_2]] &= i\hbar[\hat{J}_1, \hat{J}_3] = \hbar^2\hat{J}_2 \\
[\hat{J}_1, [\hat{J}_1, [\hat{J}_1, \hat{J}_2]]] &= \hbar^2[\hat{J}_1, \hat{J}_2] = i\hbar^3\hat{J}_3 \\
[\hat{J}_1, [\hat{J}_1, [\hat{J}_1, [\hat{J}_1, \hat{J}_2]]]] &= i\hbar^3[\hat{J}_1, \hat{J}_3] = \hbar^4\hat{J}_2 \\
&\vdots
\end{aligned}$$

And thus,

$$e^{i\phi\hat{J}_1/\hbar}\hat{J}_2 e^{-i\phi\hat{J}_1/\hbar} = \hat{J}_2\cos(\phi) - \hat{J}_3\sin(\phi).$$

Similarly we find

$$e^{i\phi\hat{J}_1/\hbar}\hat{J}_3 e^{-i\phi\hat{J}_1/\hbar} = \hat{J}_3\cos(\phi) + \hat{J}_2\sin(\phi),$$

and so on. In summary we have

$$e^{i\hat{J}_j t/\hbar}\hat{J} e^{-i\hat{J}_j t/\hbar} = R_j(t)\hat{J}, \tag{9.15}$$

where $R_j(t)$ is the rotation matrix around the axis j by an angle t.

Exercise 14. Prove that $\hat{J}_2$ and $\hat{J}_3$ have the same eigenvalues.

9.3 Spectral properties of angular momentum

We now continue to determine the eigenvalues of quantum angular momentum. Similar to the case of the harmonic oscillator, this can be done by purely algebraic methods. We start out with some considerations about orbital angular momentum, where we shall deduce that the possible eigenvalues of the components of orbital angular momentum are integer multiples of $\hbar$. We shall then move on to find that the commutation relations defining angular momentum would also allow for half-integer values. Half-integer angular momentum does indeed occur in nature, though it cannot be related to orbital angular momentum of particles, as the latter would have to be integer valued. Half-integer valued angular momentum appears as an internal degree of freedom, in the *spin* of quantum particles. We shall briefly discuss this quantum spin in section 9.5.

9.3.1 Orbital angular momentum

Let us consider the possible eigenvalues of $\hat{L}_3 = \hat{q}_1\hat{p}_2 - \hat{q}_2\hat{p}_1$. One can show that these will be given by integer multiples of $\hbar$. This is done by introducing the new set of operators $\hat{x}$ and $\hat{y}$, and $\hat{p}_x$ and $\hat{p}_y$, defined as

$$\begin{aligned}\hat{x} &= \frac{1}{\sqrt{2}}(\hat{q}_1 + \hat{p}_2), \qquad \hat{p}_x = \frac{1}{\sqrt{2}}(\hat{p}_1 - \hat{q}_2)\\ \hat{y} &= \frac{1}{\sqrt{2}}(\hat{q}_1 - \hat{p}_2), \qquad \hat{p}_y = \frac{1}{\sqrt{2}}(\hat{p}_1 + \hat{q}_2),\end{aligned}$$

which also fulfil the fundamental commutation relation of position and momenta, and rewriting $\hat{L}_3$ in terms of these operators as

$$\hat{L}_3 = \frac{1}{2}\left(\hat{p}_x^2 + \hat{x}^2\right) - \frac{1}{2}\left(\hat{p}_y^2 + \hat{y}^2\right). \tag{9.16}$$

In this way, we can interpret $\hat{L}_3$ as the difference of two harmonic oscillators $\hat{H}_x$ and $\hat{H}_y$, with masses $m = 1$ and frequencies $\omega = 1$. Remembering that the eigenvalues of the harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2$ are given by $\hbar\omega(n + \frac{1}{2})$, where n are the non-negative integers, we thus deduce that the eigenvalues of $\hat{L}_3$ are given by

$$\lambda_n = \hbar(n_x + \frac{1}{2}) - \hbar(n_y + \frac{1}{2}) = \hbar(n_x - n_y), \tag{9.17}$$

where n_j are non-negative integers. Thus, the eigenvalues of $\hat{L}_3$ are integer multiples of $\hbar$, if $\hat{L}_3$ is associated to orbital angular momentum. The same argument can be used to deduce the eigenvalues of $\hat{L}_1$ (and $\hat{L}_2$), which are also integer multiples of $\hbar$.

9.3.2 Algebraic derivation of the spectral properties

Since the three components of angular momentum do not commute, we cannot measure them simultaneously. The operator $\hat{J}^2$ commutes with all of the components, and thus, it is meaningful to talk about the total angular momentum and the component in one direction. We recall Theorem 7 from Section 4.3.2, stating that two commuting observables have simultaneous eigenvectors, and consider the simultaneous eigenvectors of $\hat{J}^2$ and one selected component of the angular momentum. In what follows we arbitrarily choose $\hat{J}_3$:

$$\hat{J}^2|\beta, m\rangle = \hbar^2\beta|\beta, m\rangle, \quad \text{and} \quad \hat{J}_3|\beta, m\rangle = \hbar m|\beta, m\rangle, \tag{9.18}$$

and ask the question: What are the possible values of β and m?

Remark 44. Due to the symmetry of the problem, the eigenvalues of $\hat{J}_1$ and $\hat{J}_2$ are the same as those of $\hat{J}_3$.

We will prove the following

Theorem 10. *The possible values of β are given by $j(j+1)$ with $2j \in \mathbb{N}$, and for each value of β m can take the values $-j, -j+1, \ldots, j-1, j$.*

We first prove

Lemma 4. *For a given β we have $m^2 \leq \beta$, that is, m is bounded from above and below.*

Proof. Assume that the states $|\beta, m\rangle$ are normalised to one. Consider the sum of the norms of the states $\hat{J}_j|\beta, m\rangle$, which are positive by definition. That is, we have

$$\sum_j \langle\beta, m|\hat{J}_j^2|\beta, m\rangle = \langle\beta, m|\hat{J}^2|\beta, m\rangle \geq 0. \tag{9.19}$$

On the other hand we have

$$\langle\beta, m|\hat{J}^2|\beta, m\rangle = \hbar^2\beta, \quad \text{and} \quad \langle\beta, m|\hat{J}_3^2|\beta, m\rangle = \hbar^2 m^2. \tag{9.20}$$

Now we don't know what the $\langle\beta, m|\hat{J}_{1,2}^2|\beta, m\rangle$ are exactly, but we do know that

$$\langle\beta, m|\hat{J}_{1,2}^2|\beta, m\rangle \geq 0, \tag{9.21}$$

and thus

$$\begin{aligned} \sum_j \langle\beta, m|\hat{J}_j|\beta, m\rangle &= \langle\beta, m|\hat{J}^2|\beta, m\rangle \\ \hbar^2\beta &\geq \hbar^2 m^2. \end{aligned} \tag{9.22}$$

□

The remainder of the proof of Theorem 10 proceeds very similarly to the case of the harmonic oscillator treated in section 5.1. We first introduce the set of adjoint operators

$$\hat{J}_\pm = \hat{J}_1 \pm \mathrm{i}\hat{J}_2. \tag{9.23}$$

We will need the commutators

$$[\hat{J}_3, \hat{J}_\pm] = \pm\hbar J_\pm \quad \text{and} \quad [\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_3, \tag{9.24}$$

and the identities

$$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_3^2 - \hbar\hat{J}_3, \quad \text{and} \quad \hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}_3^2 + \hbar\hat{J}_3. \tag{9.25}$$

Exercise 15. Verify the commutation relations (9.24) and (9.25) using the defining commutator relations (9.8).

The operators $\hat{J}_\pm$ now play the same role as the $\hat{a}^{(\dagger)}$ for the harmonic oscillator. We have the following two lemmas:

Lemma 5. *If $|\beta, m\rangle$ is an eigenvector of $\hat{J}_3$ with eigenvalue $\hbar m$, then $\hat{J}_+|\beta, m\rangle$ is either the zero vector or also an eigenvector of $\hat{J}_3$ with eigenvalue $\hbar(m+1)$.*

Lemma 6. *If $|\beta, m\rangle$ is an eigenvector of $\hat{J}_3$ with eigenvalue $\hbar m$, then $\hat{J}_-|\beta, m\rangle$ is either the zero vector or also an eigenvector of $\hat{J}_3$ with eigenvalue $\hbar(m-1)$.*

Exercise 16. Proof Lemma 5 and Lemma 6.

Since $m^2 \leq \beta$ there are either now eigenvectors at all, or there has to be a maximal value $m_{\max} = j$, for which

$$\hat{J}_+|\beta, j\rangle = 0, \tag{9.26}$$

and a minimal value $m_{\min} = k$, for which

$$\hat{J}_-|\beta, k\rangle = 0, \tag{9.27}$$

and m runs in integer values from k to j. Applying $\hat{J}_-$ to equation (9.26), and using that $\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_3^2 - \hbar\hat{J}_3$ yields

$$\begin{aligned} \hat{J}^2 - \hat{J}_3^2 - \hbar\hat{J}_3|\beta, j\rangle &= 0 \\ &= \left(\hbar^2\beta - \hbar^2 j^2 - \hbar^2 j\right)|\beta, j\rangle, \end{aligned} \tag{9.28}$$

where $|\beta, j\rangle$ is assumed not to be the zero vector. That is,

$$\beta = j^2 + j = j(j+1). \tag{9.29}$$

On the other hand, applying $\hat{J}_+$ to equation (9.27), and using that $\hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}_3^2 + \hbar\hat{J}_3$ yields

$$\begin{aligned} \hat{J}^2 - \hat{J}_3^2 + \hbar\hat{J}_3|\beta, k\rangle &= 0 \\ &= \left(\hbar^2\beta - \hbar^2 k^2 + \hbar^2 k\right)|\beta, k\rangle, \end{aligned} \tag{9.30}$$

where $|\beta, k\rangle$ is not the zero vector either, and thus

$$\beta = k^2 - k = k(k-1). \tag{9.31}$$

Combining equations (9.29) and (9.31) yields

$$k(k-1) = j(j+1), \tag{9.32}$$

which has the two possible solutions

$$k = j + 1 \quad \text{or} \quad k = -j, \tag{9.33}$$

we know, however, that k is the minimal value of m and j the maximal, that is $k \leq j$, which means we have

$$k = -j. \tag{9.34}$$

Thus we have deduced that m runs in integer steps from $-j$ to j, from which it follows that $2j$ is an integer, and the value of β is related to j by $\beta = j(j+1)$, which completes the proof of Theorem 10.

Remark 45. The eigenstates are usually labelled by the numbers j and m, rather than β and m.

Remark 46. For any given value of j there are $2j+1$ values of m.

9.4 Matrix representation in the "standard basis"

The so-called *standard basis* of angular momentum is given by the set of states $|j,m\rangle$ fulfilling

$$\begin{aligned}\hat{J}^2|j,m\rangle &= \hbar^2 j(j+1)|j,m\rangle,\\ \hat{J}_3|j,m\rangle &= \hbar m|j,m\rangle,\end{aligned} \tag{9.35}$$

with $2j \in \mathbb{N}$ and m running in integer steps from $-j$ to j. We shall now deduce the representation of the angular momentum operators in the standard basis. By definition the matrices of $\hat{J}^2$ and $\hat{J}_3$ in the standard basis are diagonal. We have

$$\langle j',m'|\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)\delta_{j'j}\delta_{m'm}, \tag{9.36}$$

and

$$\langle j',m'|\hat{J}_3|j,m\rangle = \hbar m\delta_{j'j}\delta_{m'm}, \tag{9.37}$$

We can deduce the matrix elements of $\hat{J}_1$ and $\hat{J}_2$ from those of $\hat{J}_\pm$. We know that $\hat{J}_+|j,m\rangle \propto |j,m+1\rangle$. We can find the proportionality constant from the normalisation condition. We have

$$\begin{aligned}\langle j,m+1|j,m+1\rangle &= \frac{1}{c^2}||\hat{J}_+|j,m\rangle||^2 = \frac{1}{c^2}\langle j,m|\hat{J}_-\hat{J}_+|j,m\rangle\\ &= \frac{1}{c^2}\langle j,m|\hat{J}^2 - \hat{J}_3^2 - \hbar\hat{J}_3|j,m\rangle\\ &= \frac{1}{c^2}\left(\hbar^2 j(j+1) - \hbar^2 m^2 - \hbar^2 m\right)\langle j,m|j,m\rangle\\ &= \frac{1}{c^2}\left(\hbar^2 j(j+1) - \hbar^2 m(m+1)\right)\langle j,m|j,m\rangle.\end{aligned} \tag{9.38}$$

Assuming that $\langle j,m|j,m\rangle = 1$, $|j,m+1\rangle$ is normalised if $c = \hbar\sqrt{j(j+1)-m(m+1)}$, that is,

$$\hat{J}_+|j,m\rangle = \hbar\sqrt{j(j+1)-m(m+1)}|j,m+1\rangle. \tag{9.39}$$

Similarly we find

$$\hat{J}_-|j,m\rangle = \hbar\sqrt{j(j+1)-m(m-1)}|j,m-1\rangle. \tag{9.40}$$

That is we have for the matrix elements of $\hat{J}_+$ and $\hat{J}_-$:

$$\begin{aligned}\langle j',m'|\hat{J}_+|j,m\rangle &= \hbar\sqrt{j(j+1)-m(m+1)}\delta_{j'j}\delta_{m',m+1},\\ \langle j',m'|\hat{J}_+|j,m\rangle &= \hbar\sqrt{j(j+1)-m(m-1)}\delta_{j'j}\delta_{m',m-1}.\end{aligned} \tag{9.41}$$

The matrix elements of $\hat{J}_1$ and $\hat{J}_2$ then follow from

$$\hat{J}_1 = \frac{1}{2}\left(\hat{J}_+ + \hat{J}_-\right), \quad \text{and} \quad \hat{J}_2 = \frac{1}{2\mathrm{i}}\left(\hat{J}_+ - \hat{J}_-\right). \tag{9.42}$$

The angular momentum matrices for the total angular momentum $j = \frac{1}{2}$ are given by $\hat{s}_j = \frac{\hbar}{2}\hat{\sigma}_j$, where $\hat{\sigma}_j$ denotes the Pauli matrices (8.36).

9.5 Quantum Spin

There is a quantum observable whose three components fulfil the angular momentum commutation relations, which does not describe orbital angular momentum. This observable is the so-called *spin* of a particle. It corresponds to an internal degree of freedom. The values of the spin of a particle in a given direction can be integer or half integer multiples of $\hbar$. Although it does not relate to an actual rotation or "spinning" motion of the particle, it can be transformed into orbital angular momentum. The spin is a fundamental quantity of a quantum particle, similar to for example, its mass. That is, the total value (i.e. the value of $\hat{S}^2$) is a conserved quantity.

Remark 47. There are two types of particles in nature, those with integer spin, the so-called *bosons*, and those with half-integer spin, the so-called *fermions*, which behave very differently from each other. The details of this difference could easily lead us into many more lectures and thus we will not comment further at this point.

Remark 48. The spin degree of freedom of a spin $\frac{1}{2}$ particle is described by the 2×2 representation of angular momentum, i.e. the Pauli matrices. Together with the identity matrix the Pauli matrices form a basis for all 2×2 matrices. That is, every 2×2 matrix can be written as a superposition of Pauli-matrices, and thus every quantum system with two states can be interpreted as a spin $\frac{1}{2}$ system.

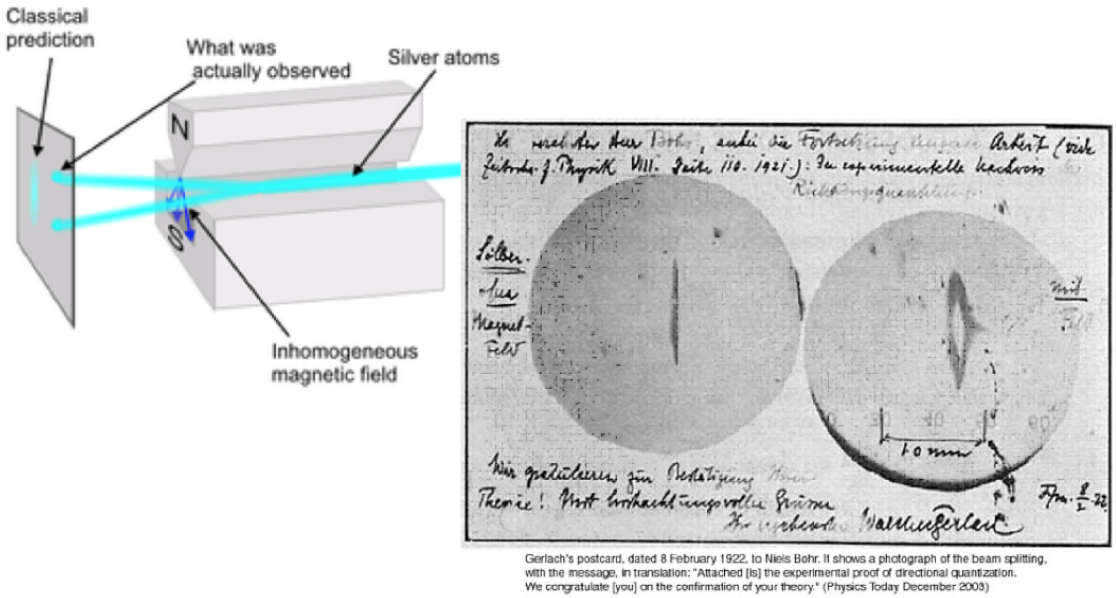


Figure 9.1: Stern-Gerlach experiment, setup, and postcard with the results from Gerlach to Bohr.

9.5.1 A short history

In 1922 a now famous experiment was performed by Stern and Gerlach, which was meant to demonstrate the quantisation of angular momentum. We now know that this was the first experimental verification of the quantum spin, even though at the time of the experiment that was not clear, and even the notion of quantum spin did not exist at the time. In the experiment, the setup of which is schematically depicted in figure 9.1 on the left, silver atoms were heated in an oven and allowed to escape and fly through an inhomogeneous magnetic field. The interaction between a charged particle with a given angular momentum and an inhomogeneous magnetic field leads to a force that is given by the so-called *magnetic moment* of the particle multiplied with the gradient of the magnetic field. The magnetic moment is proportional to the charge and the internal angular momentum of the particle. Thus, one expects that after crossing the magnetic field the silver atoms will be displaced from the straight line on which they entered the magnetic field by a distance proportional to their angular momentum. Stern and Gerlach were lucky to have chosen silver for their experiment, as the electrons in a silver atom have total orbital angular momentum of zero, and the total angular momentum of the atom is entirely due to the spin of the *outermost* electron in the atom, which has spin $\frac{1}{2}$ (that is, $j = 1/2$) and thus the beam split into two. Stern and Gerlach were aware they had measured the quantisation of angular momentum, and sent a postcard to Bohr (see figure 9.1), congratulating him on the experimental verification of his quantum theory. They were, however, not aware that they had in fact measured the internal spin degree of the electron, a

concept which didn't even exist at the time. Most certainly they had not done our calculation in Section 9.3.1, or otherwise they would have been rather surprised to find the initial beam of silver atoms had split into an even number of beams. It took until 1927 for the Stern-Gerlach experiment to be connected to the electron spin.

Uhlenbeck and Goudsmith proposed the idea of a *spin* of the electron around 1925 in their calculations of atomic spectra. At approximately the same time Pauli used the idea of a double-valued observable and introduced the *Pauli-matrices*, but said this had "nothing to do with Uhlenbeck's and Goudsmith's spin"... Not much later Dirac introduced a relativistic version of quantum theory, compatible with special relativity. In this theory, the spin comes out automatically.

Today the quantum spin is at the basis of many technologies, and gains ever more importance. Spin dynamics is the basic principle behind medical techniques such as MRI, there is an ever increasing interest in so-called *spin-tronics*, and the spin is the key ingredient (*qubit*) in quantum information.

Chapter 10

Mastery material: The Husimi distribution

10.1 Classical and quantum phase-space distributions

In classical mechanics the dynamics is conveniently represented in phase space, spanned by the classical position and momentum coordinates. Quantum mechanically, however, already the concept of a point in phase space contradicts the uncertainty principle ($\Delta p \Delta q \geq \frac{\hbar}{2}$), which is a challenge for the definition of a quantum phase space. However, there are ways to define quantum phase-space densities in analogy to classical phase-space distributions (as in statistical mechanics). None of them fulfils all the requirements we have on a classical phase-space density, $\rho(q,p)$, which are mainly

1. A classical phase-space density is real and non-negative, i.e., $\rho(q,p) \in \mathbb{R}$ and $\rho(q,p) \geq 0$ for all q, p.

2. A classical phase-space density is normalisable, i.e., the integral

$$\int \rho(q,p) \mathrm{d}p \mathrm{d}q$$

   over the whole phase space has to be finite.

3. Expectation values of functions $A(p,q)$ of position and momentum are given by phase-space integrals

$$\langle A \rangle = \int A(p,q)\rho(p,q) \mathrm{d}p \mathrm{d}q.$$

4. The p- and q-distributions are given by the marginals

$$\rho_p(q) = \int \rho(p,q) \mathrm{d}q,$$

   and

$$\rho_q(p) = \int \rho(p,q) \mathrm{d}p,$$

   respectively.

There are infinitely many choices of quantum phase-space distributions that fulfil some, but never all, of the above requirements. The ones most commonly used are the so-called Wigner and Husimi densities. Here we give a brief overview over Husimi distributions and their properties.

The Husimi distribution is defined as a projection of a state onto coherent states of a given harmonic oscillator. For this purpose we start with a summary of some of the properties of coherent states.

10.2 Coherent states

Coherent states, are minimum uncertainty states, and thus as close to the classical concept of a phase-space point as possible in quantum mechanics. They can be defined in a number of equivalent ways. One common way is as the eigenstates of the harmonic oscillator annihilation operator $\hat{a}$:

$$\hat{a}|z\rangle = z|z\rangle, \tag{10.1}$$

with eigenvalues $z \in \mathbb{C}$. In the harmonic oscillator basis $|n\rangle$ (with $\hat{H}|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle$, where $\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$), they take the form

$$|z\rangle = \mathrm{e}^{-\frac{|z|^2}{2}} \sum_n \frac{z^n}{\sqrt{n!}}|n\rangle. \tag{10.2}$$

Their position representation is given by

$$\langle x|z\rangle = \phi_z(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-\frac{m\omega}{2\hbar}(x-q)^2 + \frac{\mathrm{i}}{\hbar}px}, \tag{10.3}$$

with $z = \frac{1}{\sqrt{2\hbar}}(\sqrt{m\omega}q + \frac{\mathrm{i}}{\sqrt{m\omega}}p)$. (Verify this by applying the operator $\hat{a}$ in position representation onto the wave function (10.3)!)

The coherent states can alternatively be defined as *displaced* harmonic oscillator ground states as

$$|z\rangle = \hat{D}(z)|0\rangle, \tag{10.4}$$

where $\hat{D} = \mathrm{e}^{z\hat{a}^\dagger - z^*\hat{a}}$ is the complex displacement operator, and $|0\rangle$ is the ground state of the harmonic oscillator. The position and momentum probability distributions of this state are those of the ground state of the harmonic oscillator, only displaced to be centred around q and p respectively.

Using that $\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{-\frac{1}{2}[\hat{A},\hat{B}]}$, provided that $[\hat{A},[\hat{A},\hat{B}]] = 0 = [\hat{B},[\hat{A},\hat{B}]]$, we can rewrite $\hat{D}$ as

$$\hat{D} = \mathrm{e}^{-\frac{|z|^2}{2}}\mathrm{e}^{z\hat{a}^\dagger}\mathrm{e}^{-z^*\hat{a}}, \tag{10.5}$$

Applying this to the ground state of the harmonic oscillator and using that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \text{and} \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle,$$

we can immediately verify (10.2).

Coherent states are not orthogonal to each other. The *overlap* $|\langle z_1|z_2\rangle|^2$ of two coherent states is given by (verify this as an exercise)

$$|\langle z_1|z_2\rangle|^2 = e^{-|z_1 - z_2|^2}. \tag{10.6}$$

The coherent states form a resolution of the identity with

$$\int |z\rangle\langle z|\frac{\mathrm{d}^2 z}{\pi} = \hat{I},$$

where $\mathrm{d}^2 z = \mathrm{dRe}(z)\mathrm{dIm}(z)$.

10.3 Definition and properties of the Husimi distribution

There is a free parameter in the definition of the Husimi distribution, determined by the frequency and mass of the harmonic oscillator generating the respective coherent states, and one can adjust this parameter to yield most insights into the problem at hand. In what follows we shall for simplicity consider $m = 1 = \omega$, such that we have in the position representation

$$\langle x|z\rangle = z(x) = \left(\frac{1}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-\frac{1}{2\hbar}(x-q)^2 + \frac{\mathrm{i}}{\hbar}px}. \tag{10.7}$$

Now we identify the expectation values q and p of the coherent state with the phase-space coordinates. The Husimi distribution of a quantum state $|\psi\rangle$ is defined as

$$\rho_H(p,q) = \frac{1}{2\pi\hbar}|\langle z|\psi\rangle|^2, \tag{10.8}$$

which is equivalent to the basis expansion of $|\psi\rangle$ in the overcomplete basis of coherent states $|z\rangle$, with the normalisation factor $\frac{1}{2\pi\hbar}$.

The Husimi distribution is by definition real and positive. It is normalised if $|\psi\rangle$ is normalised, i.e.

$$\int_{-\infty}^{\infty}|\psi(x)|^2\mathrm{d}x = 1 \quad \Rightarrow \quad \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\rho_H(p,q)\mathrm{d}p\mathrm{d}q = 1. \tag{10.9}$$

The expectation values of $\hat{p}$ and $\hat{q}$ are given by

$$\langle\hat{p}\rangle = \int p\rho_H(p,q)\mathrm{d}p\mathrm{d}q, \tag{10.10}$$

and

$$\langle\hat{q}\rangle = \int q\rho_H(p,q)\mathrm{d}p\mathrm{d}q, \tag{10.11}$$

but in general

$$\langle\hat{A}\rangle \neq \int A(p,q)\rho_H(p,q)\mathrm{d}p\mathrm{d}q, \tag{10.12}$$

The position and momentum probability distributions are *not* given by the marginal distributions. Nevertheless the Husimi distribution is useful to visualise quantum mechanics in phase space and for a direct comparison to classical phase-space structures.

Exercise 17. Assume that the state $|\psi\rangle$ is normalised to one, and show that

(a) $\int \rho_H(p,q)\mathrm{d}p\mathrm{d}q = 1.$

(b) $\langle\hat{a}\rangle = \int z\rho_H(p,q)\mathrm{d}p\mathrm{d}q,$

(c) $\langle\hat{a}^\dagger\hat{a}\rangle = \int |z|^2\rho_H(p,q)\mathrm{d}p\mathrm{d}q - 1.$

10.3.1 Examples

The Husimi distribution of a coherent state $\psi(x)$ of the form

$$\psi(x) = \left(\frac{1}{\pi\hbar}\right)^{1/4}\mathrm{e}^{-\frac{1}{2\hbar}(x-q_0)^2+\frac{\mathrm{i}}{\hbar}p_0x}. \tag{10.13}$$

is given by (check!)

$$\rho_H(p,q) = \frac{1}{2\pi\hbar}\mathrm{e}^{-\frac{1}{2\hbar}\left((q-q_0)^2+(p-p_0)^2\right)}, \tag{10.14}$$

that is, a Gaussian in q and p.

The Husimi distribution of a harmonic oscillator eigenstate $|n\rangle$ is given by (check!)

$$\rho_H(p,q) = |\langle n|z\rangle|^2 = \frac{1}{2\pi\hbar}\mathrm{e}^{-|z|^2}\frac{|z|^{2n}}{n!}. \tag{10.15}$$

Three examples are depicted in the top panel of Figure 10.1. We observe that the Husimi distributions are localised around circles in phase space. These correspond to the classical phase-space trajectories with the corresponding energy.

The Husimi distribution of an arbitrary state $|\psi\rangle$ expanded in the harmonic oscillator basis $|\psi\rangle = \sum_n c_n|n\rangle$ is simply given by

$$\rho_H(p,q) = \frac{1}{2\pi\hbar}\left|\sum_n c_n\frac{z^{*n}}{\sqrt{n!}}\right|^2. \tag{10.16}$$

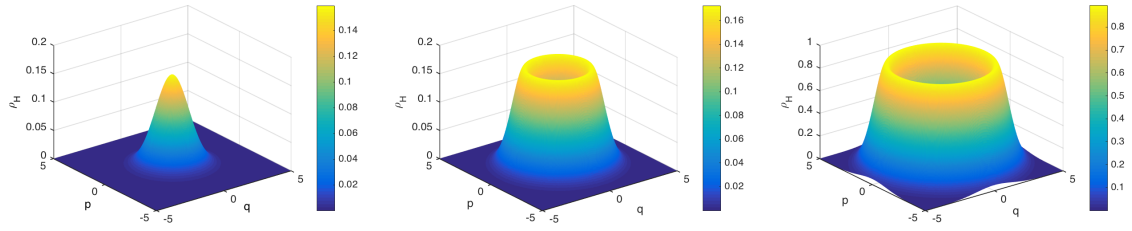


Figure 10.1: Husimi distributions of the ground state and second and fifth excited states of the harmonic oscillator.

10.3.2 Dynamics of the Husimi distribution for the Hermitian Harmonic oscillator

For a harmonic oscillator Hamiltonian, the Husimi distribution (10.16) evolves in time as

$$\rho(p,q,t) = \frac{1}{2\pi\hbar}\left|\sum_n c_n \frac{((z\mathrm{e}^{i\omega t})^*)^n}{\sqrt{n!}}\right|^2 . \tag{10.17}$$

That is, we have

$$\rho(z,t) = \rho_0(z\mathrm{e}^{i\omega t}), \tag{10.18}$$

where ρ_0 denotes the initial Husimi distribution. Hence, the dynamics of the Husimi distribution for a harmonic oscillator is a rigid rotation in phase space with frequency ω for arbitrary initial states.

10.4 SU(2) coherent states and Husimi distribution

In analogy to the coherent states of the harmonic oscillator one can define $SU(2)$ or angular momentum states for a given total angular momentum j as

$$|\zeta\rangle = N(\zeta)\mathrm{e}^{\zeta\hat{J}_+}|j,-j\rangle,$$

where $|j,-j\rangle$ is an angular momentum eigenstate with

$$\hat{J}^2|j,-j\rangle = j(j+1)|j,-j\rangle, \quad \text{and} \quad \hat{J}_3|j,-j\rangle = -j|j,-j\rangle,$$

and where $N(\zeta) = \left(1+|\zeta|^2\right)^{-j}$ is a normalisation factor. The complex variable ζ parameterises the spherical phase space. It can be related to spherical coordinates via the parameterisation $\zeta = -\mathrm{e}^{-\mathrm{i}\phi}\tan(\frac{\theta}{2})$. We can then also define a Husimi distribution on the sphere as

$$\rho_H(\theta,\phi) = \frac{1}{4\pi}|\langle\zeta|\psi\rangle|^2.$$

Exercise 18. Consider the case $j = \frac{1}{2}$.

(i) Use that $\hat{J}_+|j,m\rangle = \sqrt{j(j+1)-m(m+1)}|j,m+1\rangle$ to express the coherent states in the standard basis $|\frac{1}{2},-\frac{1}{2}\rangle$, $|\frac{1}{2},\frac{1}{2}\rangle$.

(ii) Calculate the Husimi distributions (as functions of ϕ and θ) of the two basis states.