Chapter 3

Mathematical Formalism of Quantum Mechanics

3.1 Hilbert Space

To gain a deeper understanding of quantum mechanics, we will need a more solid mathematical basis for our discussion. This we achieve by studying more thoroughly the structure of the space that underlies our physical objects, which as so often, is a vector space, the *Hilbert space.*

Definition 3.1 *A **Hilbert space** is a finite- or infinite-dimensional, linear vector space with scalar product in $\mathbb{C}$.*

The Hilbert space provides, so to speak, the playground for our analysis. In analogy to a classical phase space, the elements of the vector space, the vectors, are our possible physical states. But the physical quantities we want to measure, the observables, are now operators acting on the vectors. As mentioned in Definition 3.1, Hilbert spaces can be finite- or infinite-dimensional, as opposed to classical phase spaces (which are always $6n$-dimensional, where n is the particle number). We shall therefore investigate those two cases separately.

3.1.1 Finite–Dimensional Hilbert Spaces

In finite dimensions the vectors of a Hilbert space, denoted by $\mathcal{H}$, and the corresponding scalar products differ from the standard Euklidean case only by the choice of complex quantities $\mathbb{C}$ instead of real ones $\mathbb{R}$. It means that for vectors $x, y \in \mathcal{H}$

$$x = \begin{pmatrix} x^1 \\ \vdots \\ x^{\mathrm{n}} \end{pmatrix}, \, y = \begin{pmatrix} y^1 \\ \vdots \\ y^{\mathrm{n}} \end{pmatrix}, \quad x^{\mathrm{i}}, y^{\mathrm{i}}, \in \mathbb{C}, \tag{3.1}$$

where $\mathcal{H}$ represents the n-dimensional Hilbert space under consideration, the scalar product can be written as

$$x\,y \,=\, x_i\,y^i \,=\, \langle\,x\,|\,y\,\rangle \,=\, (x_1,\cdots,x_n)\begin{pmatrix}y^1\\\vdots\\y^n\end{pmatrix} \,=\, \sum_{i=1}^{n} x^{i*}y^i \,\in\, \mathbb{C}\,. \tag{3.2}$$

We have tried here to incorporate many different notations that are commonly used for scalar products, including the Einstein summation convention, which simply means that whenever an upper and a lower index are identical, the product is summed over. Whenever a covector[1], whose components[2] $x_i \,=\, x^{i*}$ are the complex conjugates of the corresponding vector components, is acting on a vector, with components y^i, from the left side it yields a complex number. From the above form (3.2) of the scalar product we can immediately infer the following property

$$x\,y \,=\, (y\,x)^*\,. \tag{3.3}$$

Thus the norm $\|x\|$ of a vector is guaranteed to be real and positive

$$\|x\| \,=\, \sqrt{x\,x} \,=\, (x_i\,x^i)^{1/2} \,=\, \left(\sum_{i=1}^{n} x^{i*}\,x^i\right)^{1/2} \,\in\, \mathbb{R}_{0+}\,. \tag{3.4}$$

Finally, the operators on this Hilbert space map one vector into another, i.e., they are linear transformations on the vector space, that can be represented by matrices.

$$x \,=\, A\,y \quad\Leftrightarrow\quad \begin{pmatrix}x^1\\\vdots\\x^n\end{pmatrix} \,=\, \begin{pmatrix}A_{11}&\cdots&A_{1n}\\\vdots&\ddots&\vdots\\A_{n1}&\cdots&A_{nn}\end{pmatrix}\begin{pmatrix}y^1\\\vdots\\y^n\end{pmatrix} \quad\Leftrightarrow\quad x^i \,=\, A^i{}_j\,y^j\,. \tag{3.5}$$

3.1.2   Infinite–Dimensional Hilbert Spaces

In infinite dimensions the vector space is generalized to a function space of complex valued functions, which now take the role of the state vectors[3]. The scalar product is then again defined as in Sec. 2.3.2

$$\langle\,\psi\,|\,\phi\,\rangle \,:=\, \int\limits_{-\infty}^{\infty} d^3x\,\psi^*(\vec{x})\phi(\vec{x})\,, \tag{3.6}$$

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[1]A covector is a vector of the dual vectorspace which is denoted by a row- instead of a column-vector and by lower (covariant) instead of upper (contravariant) indices for its components. The dual vectorspace is the space of linear functionals over the vectorspace, which means that in the sense of the scalar product, every vector can be mapped to a (complex) number by the action of a covector.

[2]We assume here that the basis of the covectorspace is the dual basis to our original (vectorspace) basis.

[3]They still are vectors in the abstract sense that they are elements of a vector space, but it might be misleading to view them as some sort of "arrows"

where, analogously to the finite-dimensional case, $\langle\psi|$ is a covecter (or linear functional) acting on the vector $|\phi\rangle$, which we will discuss in Sec. 3.2. The scalar product has the properties stated in Eq. (2.29) – (2.32), from which we can see that the norm of the (state) vectors, which we assume to be square integrable (and in addition normalized to one), satisfies

$$\|\psi\|^2 \ = \ \langle\,\psi\mid\psi\,\rangle \ = \ \int dx\,|\psi(x)|^2 \ = \ 1 \ < \ \infty\,. \tag{3.7}$$

The operators on this Hilbert space then map one state into the other

$$|\phi\rangle \ = \ A\,|\,\psi\,\rangle\,. \tag{3.8}$$

Another important property of the Hilbert space in infinite dimensions is its *completeness*, which we will define in the following.

Hilbert space is a *complete* function space with scalar product in $\mathbb{C}$.

Definition 3.2   *A (function) space is called* **complete** *if every Cauchy-sequence has a limit in the space.*

Definition 3.3   *A sequence $\{\psi_i\}$ is a **Cauchy sequence** if $\forall\,\epsilon\in\mathbb{R}_+$ $\exists\,N\in\mathbb{N}$ such that for all natural numbers $n,m>N$: $\|\psi_n-\psi_m\|<\epsilon$.*

This means that every sequence whose elements get even closer to each other as the sequence progresses – i.e. a Cauchy sequence – has a limit in the space, i.e., the space includes all the limits of its converging sequences and is therefore called complete. Such a property can be visualized as a space not missing any points. It guarantees that every function can be expanded with respect to the complete orthonormal basis chosen. Take for example the basis of plane waves

$$\left\{\frac{1}{\sqrt{2\pi}}e^{ikx}\right\}\,, \tag{3.9}$$

then every function $f(x)$ can[4] be expanded as

$$f(x) \ = \ \frac{1}{\sqrt{2\pi}}\int dk\,\tilde{f}(k)\,e^{ikx} \quad\text{and}\quad \tilde{f}(k) \ = \ \frac{1}{\sqrt{2\pi}}\int dx\,f(x)\,e^{-ikx}\,, \tag{3.10}$$

which is exactly the Fourier transformation of the function.

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[4]if the following integral exists

3.2   Dirac Notation

In 1930 Paul Adrian Maurice Dirac introduced in his famous book "The principles of Quantum Mechanics" the so-called "bra-ket" notation[5] which has proven very useful, easy to handle, and became therefore the standard notation in quantum mechanics. Let's discuss it in more detail.

We have already explicitly formulated the scalar product of vectors in Hilbert spaces, see Eq. (3.2) and Eq. (3.6), and we used already the notation of "bra" $\langle\,.\,|$ and "ket" $|\,.\,\rangle$. These notions can now be used independently of each other (and of the scalar product) as vectors and covectors of a Hilbert space and its dual space. We will therefore denote the vectors of a Hilbert space by the ket

$$\text{"ket"} \qquad |\,\psi\,\rangle \,\in\, \mathcal{H}\,. \tag{3.11}$$

Since the Hilbert space $\mathcal{H}$ is a vector space it has a dual vector space $\mathcal{H}^*$, which is also called the space of linear functionals over the vector space. This means that the covectors are maps from the vector space into the associated field ($\mathbb{C}$ in this case), which here is exactly provided by the "bra". So the "bra"-vectors are the elements of the dual Hilbert space[6]

$$\text{"bra"} \qquad \langle\,\phi\,| \,\in\, \mathcal{H}^*\,. \tag{3.12}$$

The (anti-)isomorphism of the Hilbert space and its dual space guarantees, that we can write down the scalar product as "bra" acting on "ket" as we are used to. Also the notation is quite unambiguous, since to every vector $|\,\psi\,\rangle$ there is exactly one dual vector $\langle\,\psi\,|$ and the bidual vector is again $|\,\psi\,\rangle$[7]. So the covectors have a one-to-one correspondence to vectors, which are our physical states. Thus we can interpret the scalar product, the "bra-ket"

$$\langle\,\phi\mid\psi\,\rangle \,=\, \int dx\,\phi^*(x)\,\psi(x) \tag{3.13}$$

as a ***transition amplitude*** from the physical state $|\,\psi\,\rangle$ to $\langle\,\phi\,|$. Technically, we turn a vector into a covector by Hermitian conjugation

$$|\,\psi\,\rangle^\dagger \,=\, \langle\,\psi\,|\,. \tag{3.14}$$

Thus, naturally, the operators on the Hilbert space are represented on the dual space by their adjoint operator (for hermitian operators these are identical)

$$A\,|\,\psi\,\rangle \quad\rightarrow\quad \langle\,\psi\,|\,A^\dagger\,. \tag{3.15}$$

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[5]Also Dirac's delta-function was introduced by him in the same book.

[6]This formulation is a little bit sloppy, but it suffices for this course. The interested reader might look up Riesz's representation theorem, which gives the mathematically exact justification.

[7]The last property is called reflexivity of the Hilbert space.

If two operators are acting on a vector, their action on the dual vector is reversed

$$A B \, | \, \psi \, \rangle \quad \rightarrow \quad \langle \, \psi \, | \, B^\dagger \, A^\dagger \, . \tag{3.16}$$

3.3 Projection Operators

The insights from the last section now allow us to try out several combinations of vectors, covectors and operators, for example,

$$A B \, | \, \psi \, \rangle \, \langle \, \phi \, | \, C \, | \, \Phi \, \rangle \, . \tag{3.17}$$

Expression (3.17) can be interpreted in different ways, either the operators B and A act successively on the vector $| \, \psi \, \rangle$ multiplied by the scalar $\langle \, \phi \, | \, C \, | \, \Phi \, \rangle$, or the vector $| \, \Phi \, \rangle$ is acted upon by the operator $A B \, | \, \psi \, \rangle \, \langle \, \phi \, | \, C$. In this last case, however, we see that we can construct operators with the combination of ket and bra, called the *exterior product*

$$\text{operator:} \quad D := | \, \psi \, \rangle \, \langle \, \phi \, | \qquad \text{adjoint operator:} \quad D^\dagger := | \, \phi \, \rangle \, \langle \, \psi \, | \, . \tag{3.18}$$

If the vectors are now chosen to be their dual vectors respectively, we get an important class of operators, the *projection operators*

$$P := | \, \psi \, \rangle \, \langle \, \psi \, | \, , \tag{3.19}$$

with the property

$$P^2 = | \, \psi \, \rangle \underbrace{\langle \, \psi \, | \, \psi \, \rangle}_{1} \langle \, \psi \, | = | \, \psi \, \rangle \, \langle \, \psi \, | = P \, . \tag{3.20}$$

3.3.1 Projectors for Discrete Spectra

The projection operators are a very important tool to expand a vector in a complete orthonormal basis $| \, \psi_\mathrm{n} \, \rangle$. We can express each vector of the Hilbert space as a linear combination of the basis vectors with complex numbers c_n

$$| \, \psi \, \rangle = \sum_n c_\mathrm{n} \, | \, \psi_\mathrm{n} \, \rangle \, . \tag{3.21}$$

By applying $\langle \, \psi_\mathrm{m} \, |$ on both sides of Eq. (3.21) we get

$$\langle \, \psi_\mathrm{m} \, | \, \psi \, \rangle = \sum_n c_\mathrm{n} \underbrace{\langle \, \psi_\mathrm{m} \, | \, \psi_\mathrm{n} \, \rangle}_{\delta_{mn}} \, . \tag{3.22}$$

Thus the coefficients c_n are given by

$$c_\mathrm{n} = \langle \, \psi_\mathrm{n} \, | \, \psi \, \rangle \, , \tag{3.23}$$

i.e. the transition amplitudes of state $|\psi\rangle$ to states $|\psi_n\rangle$. If we now insert Eq. (3.23) into Eq. (3.21)

$$|\psi\rangle = \sum_n \underbrace{|\psi_n\rangle\langle\psi_n|}_{P_n}\,\psi\rangle\,, \tag{3.24}$$

we see that for a complete set of orthonormal basis vectors the orthogonal projectors satisfy the following *completeness relation*

$$\sum_n P_n = \sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{1}\,. \tag{3.25}$$

A projection operator P_n acting on an arbitrary state $|\psi\rangle$ will thus project the state to the state $|\psi_n\rangle$ with a probability of $|\langle\psi_n|\psi\rangle|^2$. Summarizing, the P_n satisfy

$$P_n P_m = \delta_{nm} \qquad \text{and} \qquad P_n^2 = P_n\,. \tag{3.26}$$

Physically, this represents the class of projective measurements such as the measurement of the polarization of light.

Example: Polarization Filter
Consider a photon, linearly polarized along the 45°-plane (with respect to the horizontal plane). We can then describe its polarization by a state vector

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|H\rangle + |V\rangle\right)\,, \tag{3.27}$$

where $|H\rangle$ and $|V\rangle$ are the basis vectors of a 2–dimensional Hilbert space corresponding to horizontal and vertical polarization respectively. If we perform a measurement of the polarization by sending the photon through a polarization filter, e.g. in horizontal orientation, we get the measurement outcome by calculating the expectation value of the horizontal projector $|H\rangle\langle H|$. Lets first calculate the projection onto $|H\rangle$

$$|H\rangle\langle H\,|\psi\rangle = \frac{1}{\sqrt{2}}\left(|H\rangle\underbrace{\langle H\,|H\rangle}_{1} + |H\rangle\underbrace{\langle H\,|V\rangle}_{0}\right) = \frac{1}{\sqrt{2}}|H\rangle\,, \tag{3.28}$$

then we apply $\langle\psi|$ onto the left side to obtain the expectation value

$$\langle\psi\,|H\rangle\langle H\,|\psi\rangle = \frac{1}{2}\left(\underbrace{\langle H\,|\,H\rangle}_{1} + \underbrace{\langle V\,|\,H\rangle}_{0}\right) = \frac{1}{2}\,. \tag{3.29}$$

It's interesting to note that the expectation value of the projector is exactly the squared transition amplitude $\langle H\,|\psi\rangle$ – the transition probability. We conclude that the probability for the photon to pass the polarization filter is $\frac{1}{2}$.

3.3.2 Projectors for Continuous Spectra

Up to now we have only considered operators with discrete spectra, but we also have to explore projectors on, e.g., position eigenfunctions. In order to do so, we first change our notation. When working with the vectors of a system – usually, a complete orthonormal system (CONS) – the Dirac formalism allows a simplification in the notation, we may use just the label identifying the vector in the CONS, e.g.,

$$| \, \psi_n \, \rangle \quad \rightarrow \quad | \, n \, \rangle \, , \qquad | \, \psi_\xi \, \rangle \quad \rightarrow \quad | \, \xi \, \rangle \, . \tag{3.30}$$

This labeling can be applied for vectors corresponding to a discrete spectrum n as well as to a continuous spectrum ξ, as exemplified in Eq. (3.30).

Position Eigenvectors:
Let us assume vector $| \, \xi \, \rangle$ is a position eigenvector, this means

$$X \, | \, \xi \, \rangle \, = \, \xi \, | \, \xi \, \rangle \, , \tag{3.31}$$

where X is the position operator and ξ denotes the eigenvalue corresponding to the eigenvector $| \, \xi \, \rangle$. We will discuss spectra of operators and eigenvalue equations in more detail in Sec. 3.4. Projection operators are constructed in the same way as before by exterior multiplication but the corresponding properties have to be modified. The sum in the completeness relation needs to be replaced by an integral

$$\int d\xi \, | \, \xi \, \rangle \langle \, \xi \, | \, = \, \mathbb{1} \, , \tag{3.32}$$

and the orthogonality relation involves the Dirac delta function

$$\langle \, \xi' \, | \, \xi \, \rangle \, = \, \delta(\xi' - \xi) \, . \tag{3.33}$$

Now we can cast a further view on the wave functions of a Hilbert space by defining

$$\psi(x) \, := \, \langle \, x \, | \, \psi \, \rangle \quad , \quad \psi^*(x) \, = \, \langle \, \psi \, | \, x \, \rangle \tag{3.34}$$

and analogously for the basis vectors of any discrete CONS

$$\psi_n(x) \, := \, \langle \, x \, | \, n \, \rangle \quad , \quad \psi_n^*(x) \, = \, \langle \, n \, | \, x \, \rangle \, . \tag{3.35}$$

Eqs. (3.34) and (3.35) thus provide the basis-dependent notation – the wave function – of the abstract vector. That means, the abstract vector in the x-representation or the vector with respect to the chosen $| \, x \, \rangle$ basis. While the ket $| \, \psi \, \rangle$ denotes the basis-independent representation of the vector. The action of operators on the wave function is, however, independent of the basis as the operators only act on the ket. Therefore, equations such as Eq. (3.8) actually should be read as

$$A \, \psi(x) \, = \, \langle \, x | \, A \, | \, \psi \, \rangle \, = \, \langle \, x \, | \, \phi \, \rangle \, , \tag{3.36}$$

but keeping in mind that the operators act only on the ket we omit the bra $\langle \, x | $.

Let's consider now as wavefunction, the eigenfunction $\psi_\xi(x)$ of position operator X

$$\psi_\xi(x) \,=\, \langle\, x \,|\, \xi \,\rangle \,=\, \delta(x - \xi)\,, \tag{3.37}$$

which is, as expected for a position eigenfunction, perfectly localized. Technically, we need to keep in mind, that such an object is not square-integrable and thus not an element of the Hilbert space[8], but there are methods to deal with that problem, which shouldn't bother us at the moment.

Finally we can insert a CONS into Eq. (3.37) to gain the completeness relation of the wave functions in x-representation.

$$\begin{aligned}
\langle\, x \,|\, x' \,\rangle \;&=\; \langle\, x \,|\, \mathbb{1} \,|\, x' \,\rangle \,=\, \langle\, x \,|\, \sum_n |\, n \,\rangle\langle\, n \,|\, |\, x' \,\rangle \,=\, \sum_n \langle\, x \,|\, n \,\rangle\langle\, n \,|\, x' \,\rangle \;=\\
&=\; \sum_n \psi_n(x)\, \psi_n^*(x') \,=\, \delta(x - x')\,.
\end{aligned} \tag{3.38}$$

Momentum Eigenvectors:
Using again the notation of Eq. (3.30) we now write $|\, p \,\rangle$ instead of $|\, \psi_p \,\rangle$ in the eigenvalue equation for the momentum operator

$$P \,|\, p \,\rangle \,=\, p \,|\, p \,\rangle \,. \tag{3.39}$$

To be more precise we should write

$$P\,\psi_p \,=\, \langle\, x \,|\, P \,|\, p \,\rangle \,=\, \langle\, x \,|\, p \,|\, p \,\rangle\,, \tag{3.40}$$

then we can insert the x-representation of the momentum operator – the quantum mechanical correspondence (2.8) – to calculate ψ_p

$$-i\hbar\nabla\,\psi_p \,=\, p\,\psi_p\,. \tag{3.41}$$

Here ψ_p depends on x, $\psi_p \,=\, \psi_p(x)$, and we have to solve an ordinary differential equation

$$-i\hbar\frac{d}{dx}\,\psi_p \,=\, p\,\psi_p \quad\Rightarrow\quad \int\frac{d\psi_p}{\psi_p} \,=\, \frac{i}{\hbar}\,p\,dx$$

$$\ln\psi_p \,=\, \frac{i}{\hbar}\,p\,x \,+\, \text{const.} \quad\Rightarrow\quad \psi_p \,=\, \text{const.} \times e^{\,ipx/\hbar}\,. \tag{3.42}$$

The normalization of the wave function determines the constant explicitly and we can write the momentum eigenstate in the x-representation – the momentum eigenfunction – as

$$\langle\, x \,|\, p \,\rangle \,=\, \psi_p(x) \,=\, \frac{1}{\sqrt{2\pi\hbar}}\,e^{\,ipx/\hbar}\,. \tag{3.43}$$

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[8]This awkwardness can be overcome by redefining the structure of the underlying Hilbert space, which is then called the rigged Hilbert space (or Gelfand triple), but this considerations need not concern us here.

Using the completeness relation for position states, Eq (3.32), and the one for momentum eigenstates

$$\int dp \, |p\rangle\langle p| = \mathbb{1} \,, \tag{3.44}$$

we can prove the orthogonality property of the momentum and position eigenstates

$$\langle p' | p \rangle = \langle p' | \mathbb{1} | p \rangle = \langle p' | \int dx \, |x\rangle\langle x| \, |p\rangle = \int dx \, \langle p' | x \rangle\langle x | p \rangle =$$

$$= \int dx \, \psi_{p'}^*(x) \, \psi_p(x) = \frac{1}{2\pi\hbar} \int dx \, \exp\left(\frac{-ip'x}{\hbar}\right) \exp\left(\frac{ipx}{\hbar}\right) =$$

$$= \frac{1}{2\pi\hbar} \int dx \, \exp\left(\frac{i}{\hbar}(p - p')x\right) = \delta(p - p') \,, \tag{3.45}$$

$$\langle x' | x \rangle = \langle x' | \mathbb{1} | x \rangle = \langle x' | \int dp \, |p\rangle\langle p| \, |x\rangle = \int dp \, \langle x' | p \rangle\langle p | x \rangle =$$

$$= \int dp \, \psi_p(x') \, \psi_p^*(x) = \frac{1}{2\pi\hbar} \int dp \, \exp\left(\frac{ipx'}{\hbar}\right) \exp\left(\frac{-ipx}{\hbar}\right) =$$

$$= \frac{1}{2\pi\hbar} \int dp \, \exp\left(\frac{i}{\hbar}(x' - x)p\right) = \delta(x' - x) \,. \tag{3.46}$$

Expansion into a CONS:
Complete sets of orthonormal vectors are needed to expand a given vector of the Hilbert space. We start by expanding the ket

$$|\psi\rangle = \int dp \, |p\rangle\langle p | \psi \rangle = \int dp \, \tilde{\psi}(p) \, |p\rangle \,, \tag{3.47}$$

where we have used $\tilde{\psi}(p) = \langle p | \psi \rangle$ in total analogy to Eq. (3.34). The notation of the tilde for the wave function $\tilde{\psi}(p)$ explains itself once we calculate $\psi(x)$

$$\psi(x) = \langle x | \psi \rangle = \int dp \, \tilde{\psi}(p) \, \langle x | p \rangle = \int dp \, \tilde{\psi}(p) \, \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dp \, \tilde{\psi}(p) \, e^{ipx/\hbar} \,. \tag{3.48}$$

We recognize Eq. (3.48) as the Fourier transformation, i.e., the wave functions of position and of momentum space are related to each other by a Fourier transformation. It often helps to simplify complicated calculations by transforming between those spaces.

3.4 Eigenvectors and Spectral Theorem

3.4.1 Eigenvalue Equation

Eigenvalue equations play an important role in quantum mechanics. Remember that possible measurement outcomes are given by the eigenvalues of hermitian operators. This means, performing a measurement of an observable leaves[9] the system in an eigenstate of

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[9]The system stays in that particular state after the measurement, unless the state is changed by other influences (e.g. interactions, decoherence).

the corresponding operator. An arbitrary *eigenvalue equation* is of the form

$$A \,|\, j \,\rangle \;=\; \lambda_j \,|\, j \,\rangle \,, \tag{3.49}$$

where A is a linear (hermitian if we consider observables) operator with eigenvalues λ_j and corresponding eigenvectors (eigenstates) $|\, j \,\rangle$.

Let's consider a finite-dimensional Hilbert space, e.g. 2–dimensional, and an operator A acting on it. Since we are in 2 dimensions we can represent A by a 2×2 matrix and use the following identity

$$(A - \lambda_j \mathbb{1}) \,|\, j \,\rangle \;=\; 0 \,, \tag{3.50}$$

which is satisfied if the determinant of the operator acting on $|\, j \,\rangle$ vanishes

$$\det (A - \lambda_j \mathbb{1}) \;=\; 0 \,. \tag{3.51}$$

The determinant of Eq. (3.51) provides the so-called characteristic polynomial whose roots yield the possible eigenvalues of A. Making the ansatz

$$|\, i \,\rangle \;=\; \begin{pmatrix} a \\ b \end{pmatrix} \,, \qquad |\, j \,\rangle \;=\; \begin{pmatrix} c \\ d \end{pmatrix} \,, \qquad a, b, c, d \in \mathbb{C} \tag{3.52}$$

for the two (orthogonal) eigenvectors $|\, i \,\rangle$ and $|\, j \,\rangle$ and inserting them into the eigenvalue equation Eq. (3.49) gives two matrix equations, each for the pairs a, b and c, d. Two additional equations can be gained from the normalization of the vectors, which determines all constants completely

$$\langle\, i \,|\, i \,\rangle \;=\; \langle\, j \,|\, j \,\rangle \;=\; 1 \tag{3.53}$$

$$\Rightarrow \quad |a|^2 + |b|^2 \;=\; 1 \,, \quad |c|^2 + |d|^2 \;=\; 1 \,. \tag{3.54}$$

3.4.2   Spectral Theorem

The spectral theorem gives us a precise formulation of the relation between an operator and its eigenvalues.

Definition 3.4   *A linear operator A is called normal, if $A^\dagger A = A\, A^\dagger$.*

Theorem 3.1 (Spectral Theorem)
Every normal operator A can be expanded in its spectrum $\{\lambda_i\}$ by projection operators

$$A \;=\; \sum_j \lambda_j \,|\, j \,\rangle \,\langle\, j \,|$$

The theorem can also be made more specific for certain subclasses of operators, like hermitian or bounded/unbounded operators, but our formulation will suffice for this course. An important feature of the theorem, however, is its applicability to functions of operators

$$f(A) = \sum_j f(\lambda_j) \, |j\rangle \langle j| \, . \tag{3.55}$$

Example:
Consider a two-dimensional Hilbert space with an operator[10] we will call σ_x represented by the matrix

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \, . \tag{3.56}$$

We will proceed as mentioned in Section 3.4.1 to calculate the eigenvalues and eigenvectors of this matrix:

$$\det(\sigma_x - \lambda \mathbb{1}) = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1 = 0 \quad \Rightarrow \quad \lambda_{1,2} = \pm 1 \tag{3.57}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda_1 \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \quad \Rightarrow \quad a = b \tag{3.58}$$

$$|a|^2 + |b|^2 = 1 \quad \Rightarrow \quad a = b = \frac{1}{\sqrt{2}} \, , \tag{3.59}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \lambda_2 \begin{pmatrix} c \\ d \end{pmatrix} = - \begin{pmatrix} c \\ d \end{pmatrix} \quad \Rightarrow \quad c = -d \tag{3.60}$$

$$|c|^2 + |d|^2 = 1 \quad \Rightarrow \quad c = -d = \frac{1}{\sqrt{2}} \, . \tag{3.61}$$

Thus we find for the eigenvectors and for the corresponding eigenvalue equations

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \sigma_x \, |+\rangle = + \, |+\rangle \, , \tag{3.62}$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \sigma_x \, |-\rangle = - \, |-\rangle \, . \tag{3.63}$$

To construct the projectors onto $|+\rangle$ and $|-\rangle$ we first take a look at the exterior product for arbitrary components. We remember from Eq. (3.2) that the components of the covector are the complex conjugates of the ordinary vector components and that the scalar product is constructed by multiplying a row-vector with column-vector. Here the order is reversed and we get a matrix instead of a scalar

$$|\psi\rangle \langle \phi| = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \begin{pmatrix} \phi_1^* & \phi_2^* \end{pmatrix} = \begin{pmatrix} \psi_1 \phi_1^* & \psi_1 \phi_2^* \\ \psi_2 \phi_1^* & \psi_2 \phi_2^* \end{pmatrix} \, . \tag{3.64}$$

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[10]This operator is one of the Pauli matrices which occur as spin observable.

Specifically, for the projection operators P_+ and P_- we find

$$P_+ = |+\rangle\langle +| = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \qquad (3.65)$$

$$P_- = |-\rangle\langle -| = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\begin{pmatrix} 1 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \qquad (3.66)$$

The completeness and orthogonality relations then read

$$P_+ + P_- = \mathbb{1}, \qquad P_+ P_- = 0, \qquad (3.67)$$

and the spectral decomposition of σ_x (according to Theorem 3.1) is given by

$$\sigma_x = \lambda_1 P_+ + \lambda_2 P_- = P_+ - P_-. \qquad (3.68)$$

We can also calculate functions of σ_x with help of the spectral theorem, like e.g. the exponential of the matrix

$$\exp(-i\frac{\alpha}{2}\sigma_x) = \exp(-i\frac{\alpha}{2}(+1))\, P_+ + \exp(-i\frac{\alpha}{2}(-1))\, P_- =$$

$$= \frac{1}{2}\begin{pmatrix} e^{-i\frac{\alpha}{2}} + e^{i\frac{\alpha}{2}} & e^{-i\frac{\alpha}{2}} - e^{i\frac{\alpha}{2}} \\ e^{-i\frac{\alpha}{2}} - e^{i\frac{\alpha}{2}} & e^{-i\frac{\alpha}{2}} + e^{i\frac{\alpha}{2}} \end{pmatrix} = \begin{pmatrix} \cos\left(\frac{\alpha}{2}\right) & -i\sin\left(\frac{\alpha}{2}\right) \\ -i\sin\left(\frac{\alpha}{2}\right) & \cos\left(\frac{\alpha}{2}\right) \end{pmatrix}. \qquad (3.69)$$

It corresponds to the rotation of a particle with spin $\frac{1}{2}$ around the x-axis by an angle α.

3.5   Résumé: Axioms and Physical Interpretation

1. The quantum state of a system is described by the **wave function** $\psi(t,x)$. The **probability** of finding the particle in the interval $[x, x+dx]$ is supplied by $|\psi(t,x)|^2 dx$.

2. The **time evolution** of the quantum state is given by the

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

   where H denotes the Hamilton operator: $H = -\frac{\hbar^2}{2m}\Delta + V(x)$.

3. Physical quantities – **observables** – like e.g. E, P, or X, are represented by hermitian operators $A^\dagger = A$, having real eigenvalues. The eigenvalues a_n, determined by the

   eigenvalue equation $A\,|n\rangle = a_n\,|n\rangle,$

   correspond to the possible measurement outcomes.

4. Generally, a **quantum state** can be written as an

   expansion into a CONS $\quad | \psi \rangle = \sum_n c_n | n \rangle \, ,$

   where the coefficients $c_n = \langle n | \psi \rangle$ express the projections of the state $| \psi \rangle$ onto the eigenstates $| n \rangle$.

5. Experimentally, the **expectation value** of an observable is obtained by measuring a large number of identically prepared systems, each measurement provides – at random ! – a certain value a_n, which will be averaged to a mean value.

   Theoretically, the mean value $\langle A \rangle_\psi$ of an observable A in the quantum state $| \psi \rangle$ is defined by

   expectation value $\quad \langle A \rangle_\psi = \int\limits_{-\infty}^{\infty} dx \, \psi^*(t, x) \, A \, \psi(t, x) \, ,$

   and expressed in terms of eigenvalues:

   expectation value $\quad \langle A \rangle_\psi = \langle \psi | A | \psi \rangle = \sum_n |c_n|^2 \, a_n \, .$

6. The **probability** for finding an eigenvalue a_n in the quantum state $| \psi \rangle$ is given by $|c_n|^2 = |\langle n | \psi \rangle|^2$. After the measurement of A providing the value a_n the system remains in an eigenstate $| n \rangle$ – **projection postulate**.

7. The **variances** of the expectation values of operators satisfy the

   uncertainty relation $\quad \Delta A \, \Delta B \geq \frac{1}{2} |\langle [A, B] \rangle| \, ,$

   where $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 \, .$