Chapter 1

Quantum Mechanics in Hilbert Spaces

1.1 The Abstract Hilbert Space

The essential results in quantum mechanics are given through purely algebraic relations. Specific results can be derived, e.g., for vectors $\in \ell^2$ and matrices being linear maps; however, those results are essentially independent of the specific representation of the operators. For the specific results only algebraic relations between operators and abstract properties of the Hilbert space enter. This point of view allows to consider problems in full generality and then consider a specific representation of the basis vectors of the Hilbert space and the operators (e.g., matrices, differential operators).

I. The abstract Hilbert space ℓ^2 is given by a set of elements $\mathcal{H} = (|\psi\rangle, |\varphi\rangle, |\chi\rangle, \cdots)$, for which addition and multiplication with complex numbers is defined

$$|\psi\rangle + |\varphi\rangle = |\psi + \varphi\rangle \in \mathcal{H}$$
(1.1)

$$a \mid \psi \rangle = \mid a\psi \rangle \in \mathcal{H} \tag{1.2}$$

together with a scalar product

$$\langle \varphi \mid \psi \rangle \in \mathcal{C} . \tag{1.3}$$

With respect to (1.1) and (1.2), \mathcal{H} is a linear vector space, i.e.,

$$|\psi\rangle + |\varphi\rangle = |\varphi\rangle + |\psi\rangle$$

$$(|\psi\rangle + |\varphi\rangle) + |x\rangle = |\psi\rangle + (|\varphi\rangle + |x\rangle)$$

$$|\psi\rangle + |0\rangle = |\psi\rangle$$

$$|\psi\rangle + |-\psi\rangle = 0$$
(1.4)

The last two relations state the existence of a 0-vector and the existence of a negative vector with respect to $|\psi\rangle$.

$$1 | \psi \rangle = | \psi \rangle$$

$$a(b | \psi \rangle) = (ab) | \psi \rangle$$

$$(a+b) | \psi \rangle = a | \psi \rangle + b | \psi \rangle$$

$$a(| \psi \rangle + | \varphi \rangle) = a | \psi \rangle + a | \varphi \rangle$$
(1.5)

II. With respect to the scalar product, \mathcal{H} is a unitary vector space

$$\langle \psi \mid \psi \rangle \ge 0 \tag{1.6}$$

and

$$\langle \psi \mid \psi \rangle = 0 \Rightarrow \mid \psi \rangle = 0$$
 (1.7)

$$\begin{array}{lll} \langle \varphi \mid \psi \rangle &=& \langle \psi \mid \varphi \rangle^* \\ \langle \varphi \mid a\psi \rangle &=& a \langle \varphi \mid \psi \rangle \\ \langle \varphi \mid \psi_1 + \psi_2 \rangle &=& \langle \varphi \mid \psi_1 \rangle + \langle \varphi \mid \psi_2 \rangle \end{array}$$

$$(1.8)$$

Because of (1.6) a Norm can be defined

$$\parallel \psi \parallel = \sqrt{\langle \psi \mid \psi \rangle} , \qquad (1.9)$$

where the specific characteristics of the norm depend on the vector space.

One has

$$|\langle \varphi | \psi \rangle | \leq || \varphi || || \psi || || \varphi + \psi || \leq || \varphi || + || \psi ||$$

$$(1.10)$$

 $\quad \text{and} \quad$

$$\langle a\varphi \mid \psi \rangle = a^* \langle \varphi \mid \psi \rangle . \tag{1.11}$$

Further postulates are:

III. \mathcal{H} is complete.

IV. \mathcal{H} is separable.

A Hilbertspace being separable means that there exists a set of vectors dense in \mathcal{H} and countable. Let $\{|\psi_1\rangle, \dots, |\psi_k\rangle \dots\}$ be a sequence of vectors in \mathcal{H} . If we take out every vector $|\psi_k\rangle$ from this sequence, which can be represented as linear combination of the previous vector $|\psi_1\rangle, \dots |\psi_{k-1}\rangle$, then we obtain a set of linear independent vectors $\{|\varphi_1\rangle, \dots |\varphi_n\rangle \dots\}$ in which the original sequence is contained. The set of $\{|\varphi_n\rangle\}$ is via construction dense in \mathcal{H} . One can assume that $\{|\varphi_n\rangle\}$ is a set of orthogonal vectors (if not, use e.g., Gram-Schmidt orthogonalization).

$$\langle \varphi_m \mid \varphi_n \rangle = \delta_{mn} \ . \tag{1.12}$$

If $\{ | \varphi_n \rangle \}$ is dense in \mathcal{H} , we can expand every arbitrary vector according to this basis

$$|\psi\rangle = \sum_{n=1}^{\infty} |\varphi_n\rangle a_n$$
 (1.13)

and thus

$$\langle \varphi_m | \psi \rangle = \sum_{n=1}^{\infty} \langle \varphi_m | \varphi_n \rangle a_n = \sum_{n=1}^{\infty} \delta_{mn} a_n = a_m$$
 (1.14)

from which follow that each vector can be represented as

$$|\psi\rangle = \sum_{n=1}^{\infty} |\varphi_n\rangle\langle\varphi_n|\psi\rangle.$$
 (1.15)

The relation (1.15) is only valid if $\{ | \varphi_n \rangle \}$ is a complete set, and we have the completeness relation

$$\|\psi\|^{2} = \sum_{n=1}^{\infty} |\langle\varphi_{n}|\psi\rangle|^{2} . \qquad (1.16)$$

Writing the completeness relation as

$$\langle \psi \mid \psi \rangle = \langle \psi \mid \mathbf{1} \mid \psi \rangle = \sum_{n=1}^{\infty} \langle \psi \mid \varphi_n \rangle \langle \varphi_n \mid \psi \rangle$$
(1.17)

allows to represent

$$\mathbf{1} = \sum_{n=1}^{\infty} |\varphi_n\rangle\langle\varphi_n|, \qquad (1.18)$$

which is called the spectral representation of the 1-operator. The representation of the scalar product

$$\langle x \mid \psi \rangle = \sum_{n=1}^{\infty} \langle x \mid \varphi_n \rangle \langle \varphi_n \mid \psi \rangle$$
 (1.19)

through the components $\langle \varphi_n | \psi \rangle$ and $\langle \varphi_n | x \rangle$ of the vectors $| \psi \rangle$ and $| x \rangle$ with respect to the orthonormal system $\{ | \varphi_n \rangle \}$ obtained in (1.19) through "insertion" of the **1**-operator as given in (1.18). The chosen Bra- $(\langle \varphi |)$ and Ket- $(| \varphi \rangle)$ notation allows the representation of vectors in orthonormal basis systems in a very economical way.

1.2 Linear Operators in \mathcal{H}

A relation

$$A \mid \psi \rangle = \mid A\psi \rangle = \mid \psi' \rangle \tag{1.20}$$

is called linear operator in \mathcal{H} if

$$A(a \mid \psi \rangle + b \mid \varphi \rangle) = aA \mid \psi \rangle + bA \mid \psi \rangle .$$
(1.21)

In general A does not have to be defined on all vectors $\in \mathcal{H}$. In the following we will assume that $\mathcal{D}_{\mathcal{A}}$ (the range of A) is dense in \mathcal{H} .

1.2.1 Adjoint operator A^{\dagger} :

$$\langle \varphi \mid A \mid \psi \rangle = \langle A^{\dagger} \varphi \mid \psi \rangle \tag{1.22}$$

 A^{\dagger} , in general different from A, is called the to A adjoint operator if (1.22) is fulfilled. If $\mathcal{D}_{\mathcal{A}}$ is dense in $\mathcal{H}, \mathcal{A}^{\dagger}$ is uniquely defined.

1.2.2 Hermitian operators

If

$$\langle \varphi \mid A \mid \psi \rangle = \langle A\varphi \mid \psi \rangle \tag{1.23}$$

then A is called hermitian.

Comparing (1.22) and (1.23) shows that for a hermitian operator A there exists always an adjoint operator with

$$A^{\dagger} = A \tag{1.24}$$

at least on the range $\mathcal{D}_{\mathcal{A}}$ of A. It could be that A^{\dagger} defined via (1.22) exists on a larger range $\mathcal{D}_{\mathcal{A}^{\dagger}} \supset \mathcal{D}_{\mathcal{A}}$. If this is not the case, i.e., $\mathcal{D}_{\mathcal{A}^{\dagger}} = \mathcal{D}_{\mathcal{A}}$, then A is called self-adjoint. It should be mentioned that a hermitian operator only has a complete set of eigenvectors if it is self-adjoint. Since eigenvectors (or eigenfunctions) characterize quantum mechanical systems, the requirement that operators are self-adjoint (not only hermitian), if they are supported to characterize physical observables, is quite relevant.

For a self-adjoint operator we obviously have

$$(A^{\dagger})^{\dagger} = A . (1.25)$$

Properties of Hermitian Operators: The expectation value of an observable A in the state $|\psi\rangle$ (with $||\psi||=1$) is given by

$$\langle A \rangle_{\psi} = \frac{\langle \psi \mid A \mid \psi \rangle}{\langle \psi \mid \psi \rangle} = \langle \psi \mid A \mid \psi \rangle .$$
 (1.26)

In order for (1.26) to be real, one has to require A to be hermitian:

$$\langle \psi \mid A \mid \psi \rangle = \langle A\psi \mid \psi \rangle = \langle \psi \mid A\psi \rangle^*$$

from which follows that for hermitian operator A the quantity $\langle \psi \mid A \mid \psi \rangle$ is real.

If

$$A \mid \psi_a \rangle = a \mid \psi_a \rangle \tag{1.27}$$

then $|\psi_a\rangle$ is called eigenvector to A with eigenvalue a. The eigenvalues of hermitian operators are real.

Eigenvectors $|\psi_a\rangle$, $|\psi_{a'}\rangle$ of hermitian operators A to different eigenvalues $a \neq a'$ are orthogonal, i.e.,

$$\langle \psi_{a'} \mid \psi_a \rangle = 0 \tag{1.28}$$

for $a' \neq a$.

 $\mathbf{Proof:} \ \mathbf{From}$

$$A \mid \psi_a \rangle = a \mid \psi_a \rangle \tag{1.29}$$

follows

$$\langle \psi_{a'} \mid A \mid \psi_a \rangle = a \langle \psi_{a'} \mid \psi_a \rangle \tag{1.30}$$

and

$$\langle A\psi_{a'} \mid \psi_a \rangle = a' \langle \psi_{a'} \mid \psi_a \rangle = a \langle \psi_{a'} \mid \psi_a \rangle \tag{1.31}$$

and thus

$$(a'-a)\langle\psi_{a'}\mid\psi_a\rangle = 0. (1.32)$$

Since according to the assumption $a' \neq a$, i.e., $(a' - a) \neq 0$, follows that $\langle \psi_{a'} | \psi_a \rangle = 0$.

1.2.3 Isometric and unitary operators

Self-adjoint operators have a special role in quantum mechanics, since they are related to physical observables. For many theoretical considerations one needs in addition so-called **isometric** operators, which are defined as

$$\langle \Omega \varphi \mid \Omega \psi \rangle = \langle \varphi \mid \psi \rangle . \tag{1.33}$$

Because of

$$\langle \varphi \mid \Omega^{\dagger} \Omega \mid \psi \rangle = \langle \varphi \mid \psi \rangle = \langle \varphi \mid \mathbf{1} \mid \psi \rangle, \qquad (1.34)$$

they obviously fulfill

$$\Omega^{\dagger}\Omega = \mathbf{1} . \tag{1.35}$$

In finite dimensional vector spaces, the relation (1.35) would imply $\Omega\Omega^{\dagger} = \mathbf{1}$. However, for infinite dimensional vector spaces this is in general **not** the case. If an operator U fulfills

$$U^{\dagger}U = UU^{\dagger} = \mathbf{1} \tag{1.36}$$

it is called **unitary**. Another definition for an operator to be unitary can be written as

$$U^{\dagger} = U^{-1} . (1.37)$$

1.3 Matrix Representation of Linear Operators

If one has

$$A \mid \psi \rangle = \mid \psi' \rangle \tag{1.38}$$

uses the representation of the 1-operator (1.18) and multiplies from the left with $\langle \varphi_m |$, one obtains

$$\sum_{n} \langle \varphi_m \mid A \mid \varphi_n \rangle \langle \varphi_n \mid \psi \rangle = \langle \varphi_m \mid \psi' \rangle .$$
(1.39)

Here $\langle \varphi_n | \psi \rangle$ are the Fourier components of the expansion (1.15) of $|\psi\rangle$ with respect to a complete orthonormal system $\{|\varphi_n\rangle\}$. If one defines

$$\langle \varphi_m \mid A \mid \varphi_n \rangle = A_{mn} \tag{1.40}$$

then (1.39) can be written as

$$\sum_{n} A_{mn} a_n = a'_m \tag{1.41}$$

which is the form of a linear map represented by matrices. Introducing a basis in the abstract Hilbertspace assigns each vector a column vector of Fourier coefficients:

$$|\psi\rangle \longrightarrow \begin{pmatrix} \langle \varphi_1 & |\psi\rangle \\ \langle \varphi_1 & |\psi\rangle \\ \vdots \\ \langle \varphi_n & |\psi\rangle \end{pmatrix} \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$
(1.42)

and an operator corresponds to the matrix representation of a linear map

$$A \longrightarrow [\langle \varphi_m \mid A \mid \varphi_n \rangle] = [A_{mn}].$$
 (1.43)

Here all rules derived from linear algebra can be applied.

1.4 "A"-Representation

The eigenvectors $\mid \varphi_n \rangle$ of a self-adjoint operator A

$$A \mid \varphi_n \rangle = a_n \mid \varphi_n \rangle \tag{1.44}$$

for distinct eigenvalues a_n do in general **not** form a complete orthonormal system. If they do form a complete orthonormal system $\{|\psi_n\rangle\}$, then one can use those vectors as basis vectors for representing other operators.

In this particular case one can assign to an arbitrary map

$$B | \psi \rangle = | B\psi \rangle = | \psi' \rangle \tag{1.45}$$

the representation

$$\sum_{n} \langle \varphi_m \mid B \mid \varphi_n \rangle \langle \varphi_n \mid \psi \rangle = \langle \varphi_m \mid B\psi \rangle = \langle \varphi_m \mid \psi' \rangle.$$
(1.46)

It is called "A"-Representation. Specifically, the operator A is diagonal in this representation:

$$A_{mn} = \langle \varphi_m \mid A \mid \varphi_n \rangle = \delta_{mn} a_n . \tag{1.47}$$

This means: A linear operator is diagonal in its own representation. If one uses the eigenvectors of the Hamiltonian H, then this representation is called H- or energy representation.

1.5 Quantum Mechanics in Abstract Hilbert Spaces

Physical observables are assigned to self-adjoint operators, i.e., one has for position x and momentum p

$$p(t) \longrightarrow P(t)$$

$$x(t) \longrightarrow X(t)$$
(1.48)

which obey the commutation relation

$$[P,X] = \frac{\hbar}{i} \mathbf{1} . \tag{1.49}$$

All observables depending on p and x correspond to self-adjoint operators

$$A = A(P, X) , \qquad (1.50)$$

e.g., the Hamiltonian of the harmonic oscillator is given as

$$H = \frac{P^2}{2m} + \frac{m}{2} \omega^2 X^2 . \qquad (1.51)$$

A quantum mechanical state is characterized by a Hilbert space vector $|\psi\rangle$. The expectation values of operators in such a state are given as (provided $||\psi||=1$)

$$\langle A \rangle_{\psi} = \langle \psi \mid A \mid \psi \rangle . \tag{1.52}$$

The time dependence of an operator A is given through the Hamiltonian H(p, x) via

$$\dot{A} = \frac{i}{\hbar} [H, A] . \tag{1.53}$$

1.6 Root-Mean-Square Deviation

The mean value (expectation value) of an observable in a given state $|\psi\rangle$ is defined as

$$\langle A \rangle_{\psi} = \langle \psi \mid A \mid \psi \rangle \tag{1.54}$$

(with $\|\psi\|=1$). The root-mean square deviation from this expectation value is given by the mean value $(A - \langle \psi | A | \psi \rangle^2)$, i.e., through the non-negative expression

$$(\Delta A)^2_{\psi} = \langle \psi \mid (A - \langle \psi \mid A \mid \psi \rangle)^2 \mid \psi \rangle \ge 0 .$$
(1.55)

Its square root $(\Delta A)_{\psi}$ is called root-mean-square deviation or standard deviation. From (1.55) follows

$$(\Delta A)^{2}_{\psi} = \langle \psi \mid A^{2} \mid \psi \rangle - 2 \langle \psi \mid A \langle \psi \mid A \mid \psi \rangle \mid \psi \rangle + \langle \psi \mid A \mid \psi \rangle^{2}$$
(1.56)

and thus

$$(\Delta A)^2_{\psi} = \langle \psi \mid A^2 \mid \psi \rangle - \langle \psi \mid A \mid \psi \rangle^2 .$$
(1.57)

With this definition, one proves an essential theorem in quantum mechanics

The root-mean-square deviation of an observable A in the state $|\psi\rangle$ is exactly zero if $|\psi\rangle$ is eigenvector of A. The expectation value in this state corresponds to the eigenvalue.

Let $|\psi_a\rangle$ be eigenvector, i.e.,

$$A \mid \psi_a \rangle = a \mid \psi_a \rangle , \qquad (1.58)$$

then

$$\langle \psi_a \mid A \mid \psi_a \rangle = a , \qquad (1.59)$$

and thus with (1.58):

$$(\Delta A)_{\psi_a}^2 = \langle \psi_a \mid (A-a)^2 \mid \psi_a \rangle = 0 .$$
 (1.60)

Proof of inverse direction: If the root-mean-square deviation of A is zero for a state $|\psi\rangle$, then

$$0 = (\Delta A)_{\psi}^{2} = \langle \psi \mid (A - \langle \psi \mid A \mid \psi \rangle)^{2} \mid \psi \rangle$$

= $\langle (A - \langle \psi \mid A \mid \psi \rangle)\psi \mid (A - \langle \psi \mid A \mid \psi \rangle)\psi \rangle$
= $\| (A - \langle \psi \mid A \mid \psi \rangle)\psi \|^{2}$
(1.61)

and thus

$$(A - \langle \psi \mid A \mid \psi \rangle) \mid \psi \rangle = 0 .$$
(1.62)

This means that $|\psi\rangle$ is eigenvector of A with eigenvalue $\langle \psi | A | \psi \rangle$, i.e., to the mean value of A in the state $|\psi\rangle$.

If one prepares an ensemble of states experimentally in such a way that the expectation value of a state is given with zero deviation (i.e., sharp), which means that this ensemble has the same value a_n , then the ensemble is characterized by the eigenvector $|\psi_n\rangle$ via $A |\psi_n\rangle = a_n |\psi_n\rangle$.

Bound States: In quantum mechanics bound states have discrete values. If we define bound state $|\psi_n\rangle$ via

$$(\Delta H)_{\psi_n} = 0 , \qquad (1.63)$$

then, according to the above theorem, one has

$$H | \psi_n \rangle = E_n | \psi_n \rangle , \qquad (1.64)$$

i.e., bound states are obtained by solving the eigenvalue equation for the Hamiltonian H.

1.7 Uncertainty Principle

Let A and B be hermitian operators. With Schwartz' inequality follows

$$|\langle \psi | (A - \bar{A})(B - \bar{B}) | \psi \rangle| = |\langle (A - \bar{A})\psi | (B - \bar{B})\psi \rangle$$

$$\leq || (A - \bar{A})\psi || || (B - \bar{B})\psi ||$$

$$= \Delta A_{\psi} \Delta B_{\psi}$$

(1.65)

Here $\bar{A} \equiv \langle \psi \mid A \mid \psi \rangle$. The left-hand side of (1.65) can be estimated from below via

$$|Im\langle\psi|(A-\bar{A})(B-\bar{B})|\psi\rangle| \le |\langle\psi|(A-\bar{A})(B-\bar{B})|\psi\rangle| .$$
(1.66)

One also has

$$|Im \langle \psi | (A - \bar{A})(B - \bar{B}) | \psi \rangle |$$

$$= \frac{1}{2} | \langle \psi | (A - \bar{A})(B - \bar{B}) | \psi \rangle - \langle (A - \bar{A})(B - \bar{B})\psi | \psi \rangle |$$

$$= \frac{1}{2} | \langle \psi | (A - \bar{A})(B - \bar{B}) - (B - \bar{B})(A - \bar{A}) | \psi \rangle |$$

$$= \frac{1}{2} | \langle \psi | AB - BA | \psi \rangle |$$
(1.67)

From (1.65), (1.66) and (1.67) follows that

$$\frac{1}{2} |\langle \psi | [A, B] | \psi \rangle| \le (\Delta A)_{\psi} (\Delta B)_{\psi} .$$
(1.68)

Thus, if A and B do not commute, the uncertainty relation gives an estimate for the root-mean-square deviation of A and B. This is only true if $|\psi\rangle$ is not an eigenstate of A or B. If $|\psi\rangle$ would be an eigenstate of either operator, then both sides of (1.68) would vanish, and the equation would be meaningless.

Because of (1.49) one has for X and P operators

$$\frac{\hbar}{2} = \frac{1}{2} \langle \psi \mid \frac{\hbar}{i} \mathbf{1} \mid \psi \rangle \mid = \frac{1}{2} \mid \langle \psi \mid [P, X] \mid \psi \rangle \mid \\
\leq (\Delta P)_{\psi} (\Delta X)_{\psi} ,$$
(1.69)

i.e, **independent** of ψ the product of the deviations is limited from below as

$$\frac{\hbar}{2} \leq (\Delta P)_{\psi} (\Delta X)_{\psi} . \tag{1.70}$$

An immediate consequence of this relation is that neither ΔX nor ΔP vanish. Thus, according to the theorem, no eigenvectors exist for either P nor X.

Remark: It is possible to introduce eigenvectors to P and X; however, those are not normalizeable. This means they are not vectors in a Hilbertspace.

Chapter 2

Symmetries I

2.1 Constants of Motion

According to (1.53) the time dependence of an operator A is given through the Hamiltonian H(P, X) via

$$\dot{A} = \frac{\partial A}{\partial t} = \frac{i}{\hbar} [H, A] \tag{2.1}$$

The observable A is called **constant of motion** of the system, if (i) A is compatible with H, i.e.

$$[H, A] = 0 (2.2)$$

(ii)

$$\frac{\partial A}{\partial t} = 0 \tag{2.3}$$

Condition (ii) states that A does not have any **explicit** time dependence. (More on time dependence later.)

In general, symmetries or invariance properties lead to conservation laws. There are two distinct kinds of symmetries:

discrete symmetries and continuous symmetries.

Let an **infinitesimal unitary transformation** depend on a real parameter ε and vary only slightly from unity

$$\hat{U}_{\varepsilon}(\hat{G}) = \mathbf{1} + i\varepsilon\hat{G},\tag{2.4}$$

where \hat{G} is called the **generator** of the infinitesimal transformation. \hat{U}_{ε} is unitary only if ε is real and \hat{G} Hermitian

$$\hat{U}_{\varepsilon}\hat{U}_{\varepsilon}^{\dagger} = (\mathbf{1} + i\varepsilon\hat{G})(\mathbf{1} - i\varepsilon\hat{G})^{\dagger}
= \mathbf{1} + i\varepsilon(\hat{G}\hat{G}^{\dagger}) + \mathcal{O}(\varepsilon^{\epsilon})
= \mathbf{1}$$
(2.5)

only ${\bf if}$

$$\hat{G} = \hat{G}^{\dagger}.$$
(2.6)

Apply on state vector

$$\hat{U}_{\varepsilon}|\psi\rangle = (\mathbf{1} + i\varepsilon\hat{G})|\psi\rangle = |\psi\rangle + i\varepsilon\hat{G})|\psi\rangle = |\psi\rangle + \delta|\psi\rangle$$
(2.7)

Transformation of the operator A:

$$A' = \hat{U}_{\varepsilon} A \hat{U}_{\varepsilon}^{\dagger} = (\mathbf{1} + i\varepsilon(\hat{G}) A ((\mathbf{1} + i\varepsilon(\hat{G})^{\dagger}))^{\dagger}$$

$$\simeq A + i\varepsilon[\hat{G}, A]$$
(2.8)

Then A' = A only if $[\hat{G}, A] = 0$.

Finite unitary transformations can be built from infinitesimal transformations by successive application

$$\hat{U}_{\alpha}(\hat{G}) = \lim_{N \to \infty} \prod_{k=1}^{N} (\mathbf{1} + i\frac{\alpha}{N}\hat{G}) = \lim_{N \to \infty} (\mathbf{1} + i\alpha\hat{G})^{N} = e^{i\alpha\hat{G}}.$$
(2.9)

The operator \hat{U} is unitary if α is real and \hat{G} Hermitian. Then

$$\left(e^{i\alpha\hat{G}}\right)^{\dagger} = e^{-i\alpha\hat{G}} = \left(e^{i\alpha\hat{G}}\right)^{-1}.$$
(2.10)

For the transformation of an operator A one obtains

$$e^{i\alpha\hat{G}}Ae^{-i\alpha\hat{G}} = A + i\alpha[\hat{G}, A] + \frac{(i\alpha)^2}{2!}[\hat{G}, [\hat{G}, A]] + \cdots$$

= A (2.11)

only if $[\hat{G}, A] = 0$.

Consider the following examples:

1. Time Translation

 Set

$$\hat{G} \equiv \frac{1}{\hbar} H$$

$$\varepsilon = \delta t$$

$$\hat{U}_{\delta t} = \mathbf{1} + \frac{i}{\hbar} \delta t H$$
(2.12)

and apply this to a state

$$\left(\mathbf{1} + \frac{i}{\hbar}\delta tH\right)|\psi(t)\rangle = |\psi(t)\rangle - \delta t\frac{\partial}{\partial t}|\psi(t)\rangle \approx |\psi(t - \delta t)\rangle, \qquad (2.13)$$

where the explicit form of the Schrödinger equation, $H|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle$ was used. Thus one has

$$\hat{U}_{\delta t}|\psi(t)\rangle = \left(\mathbf{1} + \frac{i}{\hbar}\delta tH\right)|\psi(t)\rangle = |\psi(t - \delta t)\rangle, \qquad (2.14)$$

where H is the generator of time translations.

2. Space Translation

Consider for simplification one-dimensional space translations in x-direction. Then

$$\hat{G} \equiv \frac{1}{\hbar} \hat{P}_{x}$$
$$\hat{U}_{\varepsilon} = \mathbf{1} + \frac{i}{\hbar} \varepsilon \hat{P}_{x}$$
(2.15)

Application on a state vector yields

$$\left(\mathbf{1} + \frac{i}{\hbar} \varepsilon \hat{P}_x \right) |\psi(x)\rangle = |\psi(x)\rangle + \frac{i}{\hbar} \varepsilon \hat{P}_x |\psi(x)\rangle$$

$$= |\psi(x)\rangle + \varepsilon \frac{\partial}{\partial x} |\psi(x)\rangle$$

$$\approx |\psi(x + \varepsilon)\rangle,$$

$$(2.16)$$

where the coordinate space representation $\hat{P}_x = -i\hbar \frac{\partial}{\partial x}$ was used. For the operator X one gets

$$X' = \hat{U}_{\varepsilon}(\hat{P}_{x})X\hat{U}_{\varepsilon}^{-1}(\hat{P}_{x}) = \left(\mathbf{1} + \frac{i}{\hbar}\varepsilon\hat{P}_{x}\right)X\left(\mathbf{1} - \frac{i}{\hbar}\varepsilon\hat{P}_{x}\right)$$
$$\approx X + \frac{i}{\hbar}\varepsilon[\hat{P}_{x}, X]$$
$$= X + \varepsilon.$$
(2.17)

For finite translations one has

$$\hat{U}_{\mathbf{a}}(\mathbf{P})\psi(\mathbf{r}) = e^{\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{p}}\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{a}), \qquad (2.18)$$

where $\exp\left(\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{p}\right)$ is the generator of finite translations.

In general, symmetries and **conservation laws** are closely related. Consider the unitary transformation $\exp(i\alpha \hat{G})$. Then the Hamiltonian transforms as

$$H' = e^{i\alpha\hat{G}}He^{-i\alpha\hat{G}} = H + i\alpha[\hat{G}, H] + \frac{(i\alpha)^2}{2!}[\hat{G}, [\hat{G}, H]] + \cdots$$
(2.19)

Only if $[\hat{G}, H] = 0$ follows H' = H. We have shown before, that if $[\hat{G}, H] = 0$, then \hat{G} does not explicitly depend on the time, i.e. \hat{G} is a constant of motion. That is

$$\frac{d}{dt}\hat{G} = \frac{1}{i\hbar}[[\hat{G}, H] + \frac{\partial\hat{G}}{\partial t} = 0.$$
(2.20)

2.2 Inversion

The first example of a discrete symmetry is **inversion**.

Definition: Inversion is defined as transformation

$$\vec{x} \to \vec{x}' = -\vec{x}, \tag{2.21}$$

which means for Cartesian coordinates

$$(x, y, z) \rightarrow (x', y', z') = (-x, -y, -z)$$
 (2.22)

The geometrical interpretation is that inversion turns right-handed coordinate systems into left-handed ones and vice versa.

Studying the symmetry properties of a system under inversion means considering the behavior of the Hamiltonian under the transformation

$$H(\vec{X}, \vec{P}^2) \to H(-\vec{X}', \vec{P}^2) \equiv H'(\vec{X}', \vec{P}^2).$$
 (2.23)

Consider the kinetic energy operator $\frac{P^2}{2m}$, which is given as

$$\frac{P^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2 = -\frac{\hbar}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right).$$
(2.24)

Obviously, the kinetic energy operator is invariant if $(x, y, z) \rightarrow (-x, -y, -z)$. If one writes the Hamiltonian as

$$H(\vec{X}, \vec{P}^2) = \frac{P^2}{2m} + V(\vec{X})$$
(2.25)

one only needs to consider the transformation properties of $V(\vec{X})$. Any central potential $V(\vec{X}) \equiv V(||\vec{X}||)$ is invariant under inversion. A potential of the form

$$V(\vec{X}) \equiv V_1(|\vec{x} + \vec{a}|) + V_2(|\vec{x} - \vec{a}|), \qquad (2.26)$$

where \vec{a} is an arbitrary vector is invariant under inversion provided $V_1 = V_2$. If H is invariant under inversion, i.e.

$$H(\vec{X}, \vec{P}^2) = H(-\vec{X}, \vec{P}^2), \qquad (2.27)$$

how do wave functions $\langle \vec{x} | \phi \rangle \equiv \phi(\vec{x})$ behave?

Define an operator (parity operator) P such that

$$P\phi(\vec{x}) = \phi'(\vec{x}) = \phi(-\vec{x}).$$
(2.28)

Applying $\vec{x} \to -\vec{x}'$ gives

$$\phi(\vec{x}) = \phi(\vec{x}') = \phi'(\vec{x}').$$
(2.29)

Combining (2.28) and (2.29) gives

$$\phi(\vec{x}) = \phi'(\vec{x}') = P\phi(\vec{x}') = P\phi(-\vec{x}) = P^2\phi(\vec{x}).$$
(2.30)

Since (2.30) holds for any $|\phi\rangle$, the operator P has to fulfill

$$P^2 = 1. (2.31)$$

Let π be the eigenvalue of the operator P, then P^2 must have the eigenvalue $\pi^2 = 1$. Thus

$$P\phi(\vec{x}) = \pm \phi(\vec{x})$$

$$P\phi(\vec{x}) = \phi(-\vec{x}),$$
(2.32)

from which follows

$$\phi(-\vec{x}) = \pm \phi(\vec{x}), \tag{2.33}$$

i.e. parity eigenstates with eigenvalue +1 (-1) are even (odd) functions of \vec{x} .

¿From $P^2 = 1$ follows

$$P^{-1} = P \tag{2.34}$$

The specific choice of $\phi(\vec{x}) \equiv H(\vec{x})\psi(\vec{x})$ gives

$$P\phi(\vec{x}) = PH(\vec{x},..)\psi(\vec{x}) = H(-\vec{x},..)\psi(-\vec{x})$$

= $PH(\vec{x},..)P^{-1}P\psi(\vec{x}) = PH(\vec{x},..)P^{-1}\psi(-\vec{x}).$ (2.35)

Since $\psi(\vec{x})$ is arbitrary, one has the operator equation

$$PH(\vec{x},..)P^{-1} = H(-\vec{x},..), \qquad (2.36)$$

which leads to

$$[P, H(\vec{x}, ..)] = 0 \tag{2.37}$$

if $H(\vec{x}, ...)$ is invariant under inversion.

Thus, if the Hamiltonian is invariant under inversion, it commutes with the parity operator, and parity is a constant of motion.

Consider bound states with discrete eigenvalues as given in (1.64): If H is invariant under inversion one obtains from $H(\vec{x}, ...)\psi_n(\vec{x}) = E_n\psi_n(\vec{x})$ when applying P

$$H(\vec{x},..)\psi_n(-\vec{x}) = E_n\psi_n(-\vec{x}).$$
(2.38)

Two different cases arise:

(a) The eigenvalue E_n is non-degenerate.

Then $\psi(\vec{x})$ and $\psi(-\vec{x})$ are essentially the same function, and can differ at most by a constant factor $\tilde{\pi}$:

$$\psi(-\vec{x}) = \tilde{\pi}\psi(\vec{x}). \tag{2.39}$$

Applying $\vec{x} \to -\vec{x}$ gives

$$\psi(\vec{x}) = \tilde{\pi}\psi(-\vec{x}) = \tilde{\pi}^2\psi(\vec{x}).$$
(2.40)

Thus, $\tilde{\pi}^2 = 1$ and $\tilde{\pi} \pm 1$, which shows that $\tilde{\pi}$ is the previously introduced eigenvalue of the parity operator P, and thus

$$\psi(-\vec{x}) = \pm \psi(\vec{x}). \tag{2.41}$$

This means that the eigenfunctions to a non-degenerate eigenvalue E are either even or odd functions of \vec{x} , having either even $(\pi = +1)$ or odd $(\pi = -1)$ parity.

(b) The eigenvalue E_n is degenerate.

If (2.38) together with (1.64) holds, then any linear combination

$$a\psi(\vec{x}) + b\psi(-\vec{x}) \tag{2.42}$$

is also eigenfunction of $H(\vec{x}, ...)$ to the same eigenvalue E_n . One can use this freedom to choose linear combinations which are even or odd parity states, i.e.

$$\psi(\vec{x}) \pm \psi(-\vec{x}) \tag{2.43}$$

2.3 Ladder-Operators and the U(1) Symmetry

The Hamiltonian of the classical harmonic oscillator is a quadratic function of position and momenta. In the simplest case (provides $m = \omega 1$), it reads

$$H_{class} = \frac{1}{2} \left(p^2 + x^2 \right) , \qquad (2.44)$$

which can be decomposed as

$$H_{class} = \frac{1}{2} (x - ip)(X + ip) = a^* a , \qquad (2.45)$$

where

$$a := \frac{1}{\sqrt{2}} (x + ip) .$$
 (2.46)

In the quantum mechanics one defines a corresponding operator A

$$A := \frac{1}{\sqrt{2}} (X + iP) .$$
 (2.47)

Due to the operator character of A, the factorization of the Hamiltonian is slightly more complicated, and one obtains an additive term $\frac{1}{2}$;

$$H = \frac{1}{2} (P^2 + Q^2) = A^{\dagger} A + \frac{1}{2} \mathbf{1} . \qquad (2.48)$$

The same factorization can be applied to the differential equation for the harmonic oscillator

$$\frac{d^2 x(t)}{dt^2} + \omega^2 x(t) = 0 , \qquad (2.49)$$

where the differential operator can be decomposed as

$$\frac{d^2}{dt^2} + \omega^2 = \left(\frac{d}{dt} - i\omega\right) \left(\frac{d}{dt} + i\omega\right) . \tag{2.50}$$

Thus one obtains solutions to (2.49) if one solves one of the following first-order differential equations:

$$\left(\frac{d}{dt} - i\omega\right) x(t) = 0$$
 or $\left(\frac{d}{dt} + i\omega\right) x(t) = 0$. (2.51)

The solutions of those are

$$x(t) = x_0 e^{i\omega t}$$
 and $x(t) = x_0 e^{-i\omega t}$. (2.52)

Finally, there is a specific symmetry property in (2.44) if one considers that in the (x, p) phase space H_{class} describes the "length" of a vector in that space. Thus, H_{class} does not change if one carries out a rotation in the phase space given by

$$\begin{aligned} x' &= x \cos \alpha + p \sin \alpha \\ p' &= -x \sin \alpha + p \cos \alpha . \end{aligned}$$
(2.53)

This rotation leaves H_{class} invariant, i.e., $H_{class}(x', p') = H_{class}(x, p)$. For the quantities a from (2.45), the corresponding symmetry transformation is given by

$$a' = e^{i\alpha} a$$
 and $a'^* = e^{-i\alpha} a^*$. (2.54)

The analogous symmetry carries over into quantum mechanics, since $N = A^{\dagger}A$ is invariant under

$$A' = e^{i\alpha} A \quad \text{and} \quad A^{\dagger} = e^{-i\alpha} A^{\dagger} . \tag{2.55}$$

According to the general symmetry principle in quantum mechanics, this symmetry operation must be generated by a unitary operator. Thus, a unitary operator $U(\alpha)$ must exist, which carried A into A',

$$A' = U(\alpha)^{\dagger} A U(\alpha) . \qquad (2.56)$$

 $U(\alpha)$ can be expressed as exponential of a Hamiltonian operator

$$U(\alpha) = e^{iX(\alpha)} \tag{2.57}$$

and one has trivially for $\alpha = 0$

$$U(0) = \mathbf{1}$$
 and $X(0) = 0$. (2.58)

Important is that the transformation introduced in (2.56) forms a **group**, i.e., carrying out transformations of this kind gives another one of the same kind,

$$U(\alpha) U(\beta) = U(\alpha + \beta) . \qquad (2.59)$$

Especially, the inverse element exists:

$$U(-\alpha) = U^{-1}(\alpha) . (2.60)$$

The geometric interpretation of this group is obvious if one considers the (x, p) form of the transformation in phase space. The operator $U(\alpha)$ describes a rotation in the (x, p) plane and the group is called $O(2) \equiv$ orthogonal group in two dimensions. If one considers the complex form of (2.55), the underlying group is the unitary group with dimension d = 1, U(1).

One obtains important insight into the quantum theory if one explicitly constructs the operator $U(\alpha)$. This procedure follows the general rule that one considers first small values of the parameter α , i.e., so-called infinitesimal transformations.

Because of (2.58), one can expand

$$X(\alpha) = \alpha Y + \cdots$$
 and $(\alpha) = \mathbf{1} + i\alpha Y + \cdots$ (2.61)

Applying these to (2.56) gives

$$A' = (\mathbf{1} - i\alpha Y) A(\mathbf{1} + i\alpha Y) \approx A + i\alpha (AY - YA).$$
 (2.62)

Thus

$$A' = A + i\alpha [A, Y] + \dots \qquad (2.63)$$

This means that the infinitesimal transformation is determined by the commutator [A, Y]. Thus, Y is called the **infinitesimal generator** of the group (here U(1)). Up to now we have not used any specific properties of the group U(1). This comes into play when we expand (2.55) in powers of α

$$A' = e^{i\alpha} A \approx A + i\alpha A + \dots$$
(2.64)

Comparing (2.64) with (2.63) leads to

$$[A,Y] = A \tag{2.65}$$

which is an equation for Y, which can be solved by using

$$[N, A] = -A . (2.66)$$

The solution is (up to an additive c-number)

$$Y = N (2.67)$$

Thus, the **number operator** N is the infinitesimal generator of the group U(1).

Thus, one has a linear approximation $X(\alpha) \approx \alpha N$. Because of (2.59) $X(\alpha)$ depends linearly on α , so that $X(\alpha) = -\alpha N$ is exact. Therefore,

$$U(\alpha) = e^{-i\alpha N} \tag{2.68}$$

is an exact representation.

The results derived for the harmonic oscillator have numerous applications in modern physics, since transformations of the form (2.56) and operators with the properties of N appear in many areas of theoretical physics. Examples are particle number, electric charge, baryon number, strangeness, etc. In all cases, the quantities are "quantized," i.e., have discrete values, which are, in general, integers. Thus, we have a paradigm for understanding quantum numbers.