

Chapter 4: Mathematical Structures of Quantum Theory

- We already discussed all essential formal aspects of quantum mechanics in Chap. 2, which are sufficient to treat most quantum mechanical problems.

In this chapter we discuss further important formal aspects, mostly related to the concept of the "state", which allow for the following generalizations:

- * description of statistical ensembles of states
- * alternative formulation of time evolution: "Heisenberg picture"

4.1. States in Classical Mechanics

- We recall a number of basic aspects from theoretical classical mechanics, the Hamilton Formalism, that also play important roles in the framework of quantum theory.

We cut our discussion on formal analogies to quantum mechanics very short. See text books on more detailed and also intriguing analogies between the classical Hamilton formalism and quantum mechanics.

- Consider systems with f degrees of freedom (e.g. $f=3$ for 1 particle in 3 dimensions) with the canonical coordinates q and p in the systems phase space:

$$q = (q_1, \dots, q_f) \quad \rightarrow \text{generalized coordinates}$$

$$p = (p_1, \dots, p_f) \quad \rightarrow \text{generalized conjugate momenta}$$

Each observable A is represented by real-valued functions defined on the phase space:

$$A(q, p) = A(q_1, \dots, q_f; p_1, \dots, p_f).$$

The set of all observables defines the observable algebra.

Examples for 1 particle in 3 dimensions: phase space: $\mathbb{R}^3 \times \mathbb{R}^3 = \mathbb{R}^6$

$$(i) \text{ kinetic energy } T(\vec{x}, \vec{p}) = \frac{p^2}{2m}$$

$$(ii) i\text{-th component of angular momentum } L_i(\vec{x}, \vec{p}) = (\vec{x} \times \vec{p})_i = \epsilon_{ijk} x_j p_k$$

$$(iii) \text{ Is particle in region } \mathcal{B} \subset \mathbb{R}^3 \quad \Rightarrow \quad C_{\mathcal{B}}(\vec{x}, \vec{p}) = \begin{cases} 1, & (\vec{x}, \vec{p}) \in \mathcal{B} \\ 0, & (\vec{x}, \vec{p}) \notin \mathcal{B} \end{cases}$$

The set of all possible values in measurements of observable A is the set of values $A(q, p)$ one takes on the phase space, (spectrum of A).

- A pure state is a point (q_0, p_0) in the phase space.

In a pure state every observable has a unique value.

There is no theoretical (i.e. principle), but only practical limitation on the realization of a pure state, i.e. on the realization of many copies of the system in the pure state (q_0, p_0) .

In practice the system is in a mixed state described by a probability distribution $S(q,p)$ with

$$S(q,p) \geq 0, \quad \int dq dp S(q,p) = 1.$$

So in a practical realization of many (N) copies of the system one obtains in the measurement of observable A the expectation value

$$\langle A \rangle := \int dq dp S(q,p) A(q,p).$$

This means that if one obtains the measurements a_1, \dots, a_N one has

$$\bar{A}_N = \frac{1}{N} \sum_{n=1}^N a_n \quad \text{with} \quad \lim_{N \rightarrow \infty} \bar{A}_N = \langle A \rangle$$

Example: 1 particle in 2 dimensions

$$(1) \text{ Pure state: } S(\vec{q}, \vec{p}) = \delta^{(2)}(\vec{q} - \vec{q}_0) \delta^{(2)}(\vec{p} - \vec{p}_0)$$

$$\Rightarrow \langle A \rangle = \int d^2\vec{q} d^2\vec{p} S(\vec{q}, \vec{p}) A(\vec{q}, \vec{p}) = A(\vec{q}_0, \vec{p}_0)$$

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2 = 0$$

(2) Mixed state: Ideal gas in thermodynamic equilibrium at absolute temperature T .

The state of one single particle is described by

$$S(\vec{x}, \vec{p}) = N \underbrace{e^{-\frac{\vec{p}^2}{2mkt}}}_{\text{wave}} , \quad k = 1.38 \times 10^{-23} \text{ J K}^{-1} \quad (\text{Boltzmann constant})$$

$$\text{with} \quad \int d^3\vec{x} d^2\vec{p} S(\vec{x}, \vec{p}) = 1$$

→ We can interpret a state as a normalized, non-negative, linear functional acting on the operator algebra:

(a) Linearity: $\langle c_1 A_1 + c_2 A_2 \rangle = c_1 \langle A_1 \rangle + c_2 \langle A_2 \rangle$, for all $c_{1,2} \in \mathbb{C}$ and obs. $A_{1,2}$

(b) Positivity: $\langle A^2 \rangle \geq 0$ for all observables A

(c) Norm: $\langle 1 \rangle = 1$

We can use (a)-(c) as an abstract and generalized way to define a state, i.e. any functional satisfying (a)-(c) can be called a state.

↳ This definition of a state can be carried over almost identically to quantum mechanics. The difference is that observables in quantum mechanics are related to non-commuting objects.

→ The time evolution of a state follows the Hamilton equations

$$\dot{q} = \frac{d}{dt} q = \frac{\partial H}{\partial p}, \quad \dot{p} = \frac{d}{dt} p = -\frac{\partial H}{\partial q} \quad \text{with } H = H(q, p) \text{ the Hamilton function.}$$

Let's call the solution $q(t, q_0, p_0)$, $p(t, q_0, p_0)$ with $q(0, q_0, p_0) = q_0$, $p(0, q_0, p_0) = p_0$ then we obtain for the time-dependent expectation value

$$\langle A \rangle_t = \underbrace{\left(dq_0 dp_0 S(q_0, p_0) \right)}_{\text{time-independent state}} \underbrace{A(q(t, q_0, p_0), p(t, q_0, p_0))}_{=: A(t, q_0, p_0) \text{ time-dependent observable}} \quad (x)$$

This way to describe the time dependence is called the Heisenberg representation or the Heisenberg picture.

→ Alternative way to describe time dependence: Schrödinger picture, with time-dependent states ⊕ time-independent observables

We can switch from the Heisenberg picture to the Schrödinger picture in (x) by a change of variables: $\begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \rightarrow \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q(t, q_0, p_0) \\ p(t, q_0, p_0) \end{pmatrix} \Leftrightarrow \begin{array}{l} q_0 = q_0(t, q, p) \\ p_0 = p_0(t, q, p) \end{array}$ (Inverse exists at least for some $t > 0$)

An important aspect in the change of variables is unitarity which here is connected to the fact that the norm of the state is time-independent.

Here this directly related to the Jacobian factor is unity when changing variables from (q_0, p_0) to (q, p) , i.e. $dq_0 dp_0 = dq dp$, since the formalism does not depend on the choice of the initial time t_0 (which we picked as $t_0 = 0$).

↳ Proof: Consider the infinitesimal time $\delta t > 0$:

$$\Rightarrow q_1 = q(\delta t) = q_0 + \frac{\partial H}{\partial p} \Big|_0 \delta t, \quad p_1 = p(\delta t) = p_0 - \frac{\partial H}{\partial q} \Big|_0 \delta t$$

$$\Rightarrow \det \left(\frac{dq_1 dp_1}{dq_0 dp_0} \right) = \det \left(\begin{matrix} 1 + \frac{\partial^2 H}{\partial q \partial p} \Big|_0 \delta t & \frac{\partial^2 H}{\partial p^2} \Big|_0 \delta t \\ -\frac{\partial^2 H}{\partial q^2} \Big|_0 \delta t & 1 - \frac{\partial^2 H}{\partial q \partial p} \Big|_0 \delta t \end{matrix} \right) = 1 + O(\delta t^2) = 1$$

$|_0$: fct of q_0, p_0

because valid at any time t

$$\Rightarrow \langle A \rangle_t = \underbrace{\left(dq_0 dp_0 S(q_0(t, q, p), p_0(t, q, p)) \right)}_{=: S_t(q, p)} A(q, p)$$

$$= \underbrace{\left(dq dp \right)}_{\text{time-dependent state}} \underbrace{S_t(q, p) A(q, p)}_{\text{time-independent observable}}$$

For the time dependence of the quantum mechanical description we have used the Schrödinger picture up to now.

4.2. States in Quantum Theory

- For simplicity we consider in the following only systems for which the Hilbert space \mathcal{H} has a finite number of dimensions. For infinite-dimensional Hilbert spaces the basic formulations are still correct with obvious generalizations, but would need more involved mathematical formulations to be well-defined.
- All linear operators acting on \mathcal{H} form the operator algebra $L(\mathcal{H})$ and the Hermitian elements of $L(\mathcal{H})$ are the observables. Two observables $A, B \in L(\mathcal{H})$ do in general not commute, i.e. it is possible that $[A, B] \neq 0$.

The set of measurable values of an observable $A \in L(\mathcal{H})$ is the set of eigenvalues of A and is called the spectrum of A .

The set of eigenstates of A can be arranged such that it forms a complete orthonormal basis (CONI) of the Hilbert space \mathcal{H} .

If the spectrum of observable A is given by the eigenvalues a_1, \dots, a_m , and P_a ($i = 1, \dots, m$) are the projectors on the eigen space to eigenvalue a_i , then A can be written in the spectral representation

$$A = \sum_{i=1}^m a_i P_a$$

Recall: P_a is Hermitian and the observable to the measurement "Do we obtain in a measurement of A the value a_k ? (Yes/No)" and has the eigenvalues 1 (Yes) and 0 (No).

P_a is a projection operator, so $P_a = P_a^* P_a = P_a^2 = P_a^+$.

The possible states ω of the system are the linear functionals on the operator algebra $\omega: L(\mathcal{H}) \rightarrow \mathbb{C}$ with the properties:

(a) Linearity: $\omega(c_1 A_1 + c_2 A_2) = c_1 \omega(A_1) + c_2 \omega(A_2)$, for all $c_{1,2} \in \mathbb{C}$ and $A_{1,2} \in L(\mathcal{H})$

(b) Positivity: $\omega(A^* A) \geq 0$ for all $A \in L(\mathcal{H})$ [note: $\omega(A^* A) \in \mathbb{R}_0^+$]

(c) Norm: $\omega(\mathbb{1}) = 1$

The value $\omega(A)$ is the expectation value $\langle A \rangle$ in a measurement of A on a large number of copies of the system in the state ω .

The positive real number $p_\alpha := \omega(P_\alpha) = \omega(P_\alpha P_\alpha) = \omega(P_\alpha^+ P_\alpha) \geq 0$

is the probability to obtain the value a_α in a measurement of observable A when the system is in state ω . This is consistent with

$$\sum_{\alpha=1}^m p_\alpha = \sum_{\alpha=1}^m \omega(P_\alpha) \stackrel{(a)}{=} \omega\left(\sum_{\alpha=1}^m P_\alpha\right) \stackrel{\text{completeness}}{=} \omega(\mathbb{1}) = 1 \quad (\text{probability for any value } a_\alpha)$$

$$\omega(A) = \omega\left(\sum_{\alpha=1}^m a_\alpha P_\alpha\right) \stackrel{(a)}{=} \sum_{\alpha=1}^m a_\alpha \omega(P_\alpha) = \sum_{\alpha=1}^m a_\alpha p_\alpha$$

Different types of states:

(1) **Pure state**: Let be $|4\rangle \in \mathcal{X}$ a normalized state ($\langle 4|4\rangle = 1$), then the functional $w(A) = \langle 4|A4\rangle$ for all $A \in L(\mathcal{X})$ defines a pure state satisfying (a)-(c). The set of states $\{e^{i\alpha}|4\rangle, \alpha \in \mathbb{R}\}$ are physically equivalent and called ray of state $|4\rangle$ in \mathcal{X} .

(2) **Mixed state**: Let $\omega_1, \omega_2, \dots, \omega_r$ be pure states (related to $|4_1\rangle, \dots, |4_r\rangle$) and $p_1, p_2, \dots, p_r > 0$ with $\sum_{i=1}^r p_i = 1$, then

$$\omega = \sum_{i=1}^r p_i \omega_i \text{ is also a state.}$$

(We then have $\omega(A) = \sum_{i=1}^r p_i \langle 4_i|A4_i\rangle$ for all $A \in L(\mathcal{X})$). In general:

There is no state $|4\rangle \in \mathcal{X}$, for which we have $\omega(A) = \langle 4|A4\rangle$ for all $A \in L(\mathcal{X})$

States which have this property are called mixed states.

→ Standard form for pure and mixed states : Density operator

Consider the arbitrary orthonormal basis $\{|e_1\rangle, \dots, |e_n\rangle\}$ ($\dim(\mathcal{X}) = n$) of \mathcal{X} . The operation of any operator $A \in L(\mathcal{X})$ can be written in terms of the matrix elements $A_{ek} := \langle e_k|A|e_k\rangle$.

Due to linearity (point (a)) $\omega(A)$ can be written as $\omega(A) = \sum_{k \in \mathcal{E}} S_{ek} A_{ek}$.

We can interpret the S_{ek} as matrix elements $S_{ek} = \langle e_k|S|e_k\rangle$ of the abstract operator S , which fully characterize the state ω . What are the properties of S ?

$$\begin{aligned} \omega(A) &= \sum_{k=1}^n \sum_{e=1}^n \langle e_k|S|e_k\rangle \times e_k|A|e_k\rangle \\ &\stackrel{\text{Commutativity}}{=} \sum_{k=1}^n \langle e_k|S A e_k\rangle =: \text{Tr}(S A) \end{aligned}$$

Note: The trace of any matrix is always basis-independent!

↪ Take projection operator $A = |4\rangle\langle 4|$ (with arbitrary normalized state $|4\rangle$) as the observable: so $A = A^\dagger$, $A^\dagger A - A$. \Rightarrow For any normalized $|4\rangle$ we have

$$\begin{aligned} \langle 4|S4\rangle &= \sum_{k=1}^n \langle 4|e_k\rangle \times e_k|S|4\rangle = \sum_{k=1}^n \langle 4|e_k\rangle \times |4\rangle\langle 4|e_k\rangle = \omega(A) \\ &= \omega(A^\dagger A) \stackrel{(b)}{\geq} 0 \quad \text{for all } |4\rangle \in \mathcal{X}, \text{ so } S \text{ is called a positive operator.} \end{aligned}$$

↪ For positive operators the following statements are equivalent:

1.) $\langle 4|S4\rangle \geq 0 \quad \text{for all } |4\rangle \in \mathcal{X}$

2.) S is Hermitian and all its eigenvalues are ≥ 0

3.) There exists an operator $A \in L(\mathcal{X})$, with $S = A^\dagger A$

Each of these statements is incorporating properties (a) and (b) of the state functional ω . Property (c) will come below.

Proof in circle:

1. \Rightarrow 2. Let $|1\rangle_c$ and $|2\rangle_c$ be two normalized and orthogonal states

$$\Rightarrow \langle 1\rangle_c \langle 2| S(1\rangle_c + 2\rangle_c) = S_{11} + S_{22} + S_{12} + S_{21} = 0 \Rightarrow \text{Im}(S_{12} + S_{21}) = 0$$

$$\langle 1\rangle_c \langle 2| S(1\rangle_c + i2\rangle_c) = S_{11} + S_{22} + iS_{12} - iS_{21} = 0 \Rightarrow \text{Re}(S_{12} - S_{21}) = 0$$

$$\Rightarrow S_{12} = S_{21}^* \Rightarrow S = S^+ \quad (\text{since we can run } |1\rangle_c \text{ and } |2\rangle_c \text{ through a CONS})$$

Let $|X_k\rangle$ be an eigenstate to S with eigenvalue S_k , then

$$\langle X_k | S | X_k \rangle = S_k \langle X_k | X_k \rangle \geq 0 \Rightarrow S_k \geq 0 \text{ for all } k$$

◻

2. \Rightarrow 3. Due to the spectral theorem there is a CONS $\{|X_1\rangle, \dots, |X_n\rangle\}$ of eigenstates of S with eigenvalues $S_k \geq 0$, and we can write

$$S = \sum_{k=1}^n S_k |X_k\rangle \langle X_k|$$

We can now define the operator $\sqrt{S} := \sum_{k=1}^n \sqrt{S_k} |X_k\rangle \langle X_k|$, for which we have
 $(\sqrt{S})^* \sqrt{S} = \sqrt{S} \sqrt{S} = S$

◻

3. \Rightarrow 1. For any $|A\rangle \in \mathcal{X}$ we have $\langle A | S | A \rangle = \langle A | A^\dagger A | A \rangle = \langle A^\dagger A | A \rangle \geq 0$

◻

Let $\{|X_1\rangle, \dots, |X_n\rangle\}$ be a CONS of eigenstates of S with eigenvalues $S_k \geq 0$

$$\Rightarrow \omega(A) = \text{Tr}(S) = 1 \Rightarrow \sum_{k=1}^n S_k = 1$$

The density operator $S = \sum_{k=1}^n S_k |X_k\rangle \langle X_k|$ with $S_k \geq 0$ and $\text{Tr}(S) = \sum_{k=1}^n S_k = 1$ with $\omega(A) := \text{Tr}(SA)$ for all $A \in L(\mathcal{X})$ provides the general standard form representing any possible state.

Mixed state: If at least 2 of the S_k are non-zero then S represents the statistical mixture of the system being in either of the pure states $|X_k\rangle$ with probability S_k . We have $S^2 = S$. This is consistent with

$$\omega(A) = \text{Tr}(SA) = \sum_{k=1}^n \langle X_k | S | X_k \rangle = \sum_{k=1}^n S_k \underbrace{\langle X_k | A | X_k \rangle}_{\substack{\text{Classical statistical probability} \\ \text{of the system to be in state } |X_k\rangle}}$$

Quantum mechanical expectation value
for measurement of A in the state $|X_k\rangle$

Pure state: If exactly one S_k is non-zero, then $S = |X_k\rangle \langle X_k|$ represents a system being with probability 1 in the (normalized) state $|A\rangle \in \mathcal{X}$. Then S_A is a projector with $S_A^2 = S_A$ and we have

$$\omega_A(A) = \sum_{k=1}^n \langle X_k | A^\dagger A | X_k \rangle = \sum_{k=1}^n \langle A | X_k \rangle \langle X_k | A \rangle = \langle A | A \rangle$$

as it should be.

Example:

(1) State of maximal mixing

Let be $\dim(\mathcal{H}) = n$, then $S = \frac{1}{n} \mathbf{1}$ has only the eigenvalue $\frac{1}{n}$ where all states are eigenstates. For any given COWB this state represents a statistical mixture where each state of the COWB has exactly the same probability $\frac{1}{n}$.

(2) State in thermodynamical equilibrium

Let a system have the hamiltonoperator H , which is in thermodynamical equilibrium with an external heat bath with absolute temperature T :

$$S = \frac{e^{-H/kT}}{\text{Tr}(e^{-H/kT})}$$

Let $\{|e_1\rangle, \dots, |e_n\rangle\}$ be a COWB of energy eigenstates with $H|e_x\rangle = E_x|e_x\rangle$, $x = 1, \dots, n$, then the spectral representation of S has the form

$$S = \frac{1}{Z} \sum_{x=1}^n e^{-E_x/kT} |e_x\rangle \langle e_x|, \quad Z = \sum_{x=1}^n e^{-E_x/kT}$$

(3) Pure vs. mixed state (part A)

Let $|e_1\rangle$ and $|e_2\rangle$ be two orthonormal states.

(a) pure state $|e\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle + |e_2\rangle)$

$$\rightarrow S_p = |e\rangle \langle e| = \frac{1}{2} |e_1\rangle \langle e_1| + \frac{1}{2} |e_2\rangle \langle e_2| + \underbrace{\frac{1}{2} (|e_1\rangle \langle e_2| + |e_2\rangle \langle e_1|)}_{\substack{\text{"off-diagonal terms"} \\ \text{"interference terms"}}}$$

(b) mixed state: 50% $|e_1\rangle$ and 50% $|e_2\rangle$

$$\rightarrow S_{50\%} = \frac{1}{2} |e_1\rangle \langle e_1| + \frac{1}{2} |e_2\rangle \langle e_2|$$

→ General uncertainty relation for arbitrary states

The properties (a) - (c) of arbitrary states are sufficient to show that for arbitrary observables A, B

$$\Delta_w A \Delta_w B \geq |\omega(\frac{1}{2}[A, B])| \quad \text{with}$$

$$(\Delta_w X)^2 = \omega((X - \omega(X)\mathbf{1})^2) = \omega(X^2) - (\omega(X))^2, \quad X = A, B$$

So the general uncertainty relation has the same form for pure and mixed states.

→ Pure vs. mixed states (part B) → see part A above

Very interesting is the following fact: Assume that $|4_1\rangle$ and $|4_2\rangle$ are eigenstates of observable A to the same eigenvalue, i.e. $A|4_{1,2}\rangle = \alpha|4_{1,2}\rangle$. Then the pure state S_A and the mixed state S_{mixed} will always give the value α in measurements of A, with $\Delta_{\text{w}}A = 0$.

It is possible to construct infinitely many such different states that always yield the same value α in a measurement of A, with $\Delta_{\text{w}}A = 0$.

$$S_{\text{pure}} = (\alpha^* \langle 4_1 | + \beta^* \langle 4_2 |)(\alpha |4_1\rangle + \beta |4_2\rangle) \quad \text{with } \alpha, \beta \in \mathbb{C}, |\alpha|^2 + |\beta|^2 = 1$$

$$S_{\text{mix}} = p_1 |4_1\rangle \langle 4_1| + p_2 |4_2\rangle \langle 4_2|, \quad \text{with } 0 \leq p_{1,2} \leq 1, \quad p_1 + p_2 = 1$$

So making only measurements of A is not sufficient to see that these states are quantum mechanically different. One needs to carry out measurements of at least another observable B for which $|4_1\rangle$ and $|4_2\rangle$ can yield different values.

→ For measurements of observable A we have $\Delta_{\text{w}}A = 0$ if and only if $AS = SA = \alpha S$ where α is the value that is (always) measured.

The theorem also illustrates why in quantum physics it is impossible to have measurements that yield unique (sharp) values for all observables (as is in principle possible in classical mechanics): For any given density matrix S it is always possible to find an observable A such that $[A, S] \neq 0$.

Proof: Take observable $B = I^2$ with $\omega(I^2) = 0$. Let be $S = \sum_{k=1}^n S_k |x_k\rangle \langle x_k|$, $\{|x_k\rangle\}$ is CONS.

$$\Leftrightarrow 0 = \text{Tr}(S I^2) = \sum_{k=1}^n S_k \langle x_k | I^2 | x_k \rangle = \sum_{k=1}^n S_k \langle I x_k | I x_k \rangle$$

$$\Leftrightarrow B|x_k\rangle = 0 \quad \text{für alle } S_k \neq 0$$

$$\Leftrightarrow \langle x_l | B | x_k \rangle = \langle x_k | B | x_l \rangle = 0, \quad l=1, \dots, n \quad \text{für alle } S_k \neq 0 \quad \Leftrightarrow BS = SB = 0$$

$$\hookrightarrow \text{Take } B = A - \omega(A) \text{ then } BS - SB = 0 \Leftrightarrow AS - SA = \omega(A)S \quad \square$$

→ State reduction: state collapse

Ideal measurement in classical physics: The system is just observed and not affected by the process of measurement.

Ideal measurement in quantum physics: The measurement process in general affects the state of the system, since the state of the system collapses to the projection of the original state on the eigenspace corresponding to the measured value.

Comment:

"Ideal" means that the particle is not destroyed by the measurement process or turned into a different number of particles.

Description of state collapse in an ideal measurement: (Neumann's Projection Theorem)

Observable: $A = \sum_{k=1}^m \alpha_k P_k$, $\alpha_k + \alpha_\ell$ for $k \neq \ell$, P_k : projects on eigenspace to eigenvalue α_k

State prior to measurement: S

State after the measurement of the value α_k : $S' = \frac{P_k S P_k}{\text{Tr}(P_k S P_k)}$

↳ The functional $\omega(O)$ of any observable $O \in L(\mathcal{H})$ related to the reduced state has the form

$$\omega'(O) = \text{Tr}(S' O) = \frac{\text{Tr}(P_k S P_k O)}{\text{Tr}(S P_k)} = \frac{\text{Tr}(S P_k O P_k)}{\text{Tr}(S P_k)} = \frac{\omega(P_k O P_k)}{\omega(P_k)}$$

$$\begin{aligned} & \text{Tr}(P_k S P_k) \\ &= \text{Tr}(S P_k^2) \\ &= \text{Tr}(S P_k) \end{aligned}$$

Educational exercises:

- Show that S' is indeed a density operator.
- Show that $O \rightarrow \omega'(O)$ indeed has the properties of a state functional.

4.3. Schrödinger Picture vs. Heisenberg Picture

→ We assume: Hamilton operator H is time-independent

→ Schrödinger picture $H_S \equiv H$ (subscript "S" for "Schrödinger picture")

- ☒ Time dependence contained in the states
- ☒ Observables are time independent.

Time evolution of states given by the Schrödinger equation: $i\hbar \frac{d}{dt} |\psi_S(t)\rangle = H_S |\psi_S(t)\rangle$

Solution: $|\psi_S(t)\rangle = U_S(t) |\psi_S(0)\rangle$, $U_S(t) = \exp(-iH_S t/\hbar)$

unitary time-evolution operator: $U_S(t) = U_S^\dagger(t) = \exp(iH_S t/\hbar)$

The unitarity of $U_S(t)$ is directly related to

- (1) time independence of the norm of $|\psi_S(t)\rangle$
- (2) conservation of the total probability
- (3) conservation of the particle number

$$\left. \begin{array}{l} (1) \langle \psi_S(t) | \psi_S(t) \rangle = \langle \psi_S(0) | \psi_S(0) \rangle \\ (2) \langle \psi_S(t) | \psi_S(t) \rangle = \langle \psi_S(0) | \psi_S(0) \rangle \end{array} \right\}$$

Time evolution of the density operator:

$$S_S(t) = U_S(t) S_S(0) U_S^\dagger(t)$$

↳ Differential equation: $i\hbar \frac{d}{dt} S_S(t) = [H_S, S_S(t)]$

$$\text{Derivation: } \frac{d}{dt} U_S(t) = -\frac{i}{\hbar} H U_S(t) = -\frac{i}{\hbar} U_S(t), \quad \frac{d}{dt} U_S^\dagger(t) = \frac{i}{\hbar} H U_S^\dagger(t) = \frac{i}{\hbar} U_S^\dagger(t) H$$

$$\Rightarrow \frac{d}{dt} S_S(t) = -\frac{i}{\hbar} (H S_S(t) - S_S(t) H)$$

Observables: time-independent Hermitian operators in $L(\mathcal{H})$

Time dependence of expectation value of observable A_S : $\omega_t(A_S) = \text{Tr}(S_S(t) A_S)$

→ Heisenberg picture: (subscript "H" for Heisenberg picture)

- ☒ Time-dependence contained in the observables.
- ☒ States are time-independent.

We use the trace identity $\text{Tr}(XYZ) = \text{Tr}(ZXY) = \text{Tr}(YZX)$ to write

$$\omega_t(A) = \text{Tr}(S_S(t) A_S) = \text{Tr}(U_S(t) S_S(0) U_S^\dagger(t) A_S)$$

$$= \text{Tr}(S_S(0) U_S^\dagger(t) A_S U_S(t))$$

$$\omega_t(A) = \text{Tr}(S_H A_H(t)) \quad \text{with } S_H = S_S(0), \quad A_H(t) = U_S^\dagger(t) A_S U_S(t)$$

↙ ↘
time-independent state time-dependent observable

$$= U_S^\dagger(t) A_H(0) U_S(t)$$

Heisenberg evolution equations: $\frac{d}{dt} A_n(t) = \frac{i}{\hbar} [H, A_n(t)]$

We find: $\frac{d}{dt} A_n(t) = 0 \Leftrightarrow [H, A_n(t)] = 0 \Leftrightarrow [H, A_s] = 0$

Observables that commute with the Hamilton operator do not change with time.
Such observables are called conserved quantities.

↳ The Hamilton operator $H_n(t) = H_n(0) = H_0 = H$ is time-independent which corresponds to energy conservation.

↳ The canonical commutation relations for x and p lead to the fact that the Heisenberg evolution equations for $X_n(t)$ and $P_n(t)$ have the same form as for classical mechanics:

Example: Particle in a potential $V(x)$

$$H = H_n(t) = \frac{P_n^2(t)}{2m} + V(X_n(t)) = H_n(0) = \frac{P_n^2(0)}{2m} + V(X_n(0))$$

$$\begin{aligned} \dot{X}_n(t) &= \frac{i}{\hbar} [H_n(t), X_n(t)] = \frac{i}{\hbar} \left[\frac{P_n^2(t)}{2m} + V(X_n(t)), X_n(t) \right] \\ &= \frac{i}{\hbar} \left[\frac{P_n^2(t)}{2m}, X_n(t) \right] \end{aligned}$$

$$\begin{aligned} [X_n(t), P_n(t)] &= [U_s^\dagger(t) X_s U_s(t), U_s^\dagger(t) P_s U_s(t)] = U_s^\dagger(t) \underbrace{[X_s, P_s]}_{i\hbar \mathbb{1}} U_s(t) \\ &= i\hbar \mathbb{1} \quad \Rightarrow [P^2, X] = P[P, X] + [P, X]P = -2i\hbar P \end{aligned}$$

$$\Rightarrow \dot{X}_n(t) = \frac{P_n(t)}{m}$$

$$\dot{P}_n(t) = \frac{i}{\hbar} [H_n(t), P_n(t)] = \frac{i}{\hbar} [V(X_n(t)), P_n(t)] \quad [V(x), P] = i\hbar V'(x)$$

$$\dot{P}_n(t) = -V'(X_n(t))$$

4.4. Hilbert Space with Two Dimensions

→ The simplest non-trivial Hilbert space has 2 dimensions. It carries almost all essential features of general quantum mechanical Hilbert spaces and has important physical applications (\rightarrow spin $\frac{1}{2}$ particles, optics, ...).

→ We pick a CWS $\{|1\rangle, |1\rangle\}$ of \mathcal{H} : $\langle 1|1\rangle = \langle 1|1\rangle = 1$, $\langle 1|1\rangle = 0$, (orthonormality)

$$|1\rangle \times |1\rangle + |1\rangle \times |1\rangle = \mathbb{1} = \mathbb{1}_{2 \times 2} \quad (\text{completeness})$$

All $|x\rangle \in \mathcal{H}$ are a linear combination of $|1\rangle$ and $|1\rangle$: $|x\rangle = |1\rangle \underbrace{\langle 1|x\rangle}_{c_1} + |1\rangle \underbrace{\langle 1|x\rangle}_{c_2} = c_1|1\rangle + c_2|1\rangle$, $c_{1,2} \in \mathbb{C}$

Scalar product: $\langle x|1\rangle = b_1^* c_1 + b_2^* c_2$ for $|x\rangle = b_1|1\rangle + c_2|1\rangle$

↳ Every state can be uniquely written as 2-dim complex vector: $|x\rangle \in \mathcal{H} \leftrightarrow \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, c_{1,2} \in \mathbb{C}$

with the scalar product: $\langle x|1\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}^* \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = (b_1^*, b_2^*) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = b_1^* c_1 + b_2^* c_2$

This complex vector space is called \mathbb{U}_2 .

→ An arbitrary linear operator $A \in L(\mathcal{H})$ can be written in terms of its matrix elements

$$A = A_{11}|1\rangle \langle 1| + A_{12}|1\rangle \langle 1| + A_{21}|1\rangle \langle 1| + A_{22}|1\rangle \langle 1|$$

which also has the matrix representation
with respect to the CWS $\{|1\rangle, |1\rangle\}$

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad A_{12} \in \mathbb{C} \quad \left. \begin{array}{l} \text{arbitrary complex} \\ 2 \times 2 \text{ matrix} \end{array} \right.$$

The Hermitian matrices $\{\mathbb{1}, \vec{\sigma}\}$ form a complete basis of all complex 2×2 matrices A

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \leftarrow \vec{\sigma}: \text{Pauli matrices}$$

$a_0, a_k \in \mathbb{R}$
for observables

$$A = a_0 \mathbb{1} + \sum_{k=1}^3 a_k \sigma_k = a_0 \mathbb{1} + \vec{a} \vec{\sigma} \quad \text{with } a_0, a_k \in \mathbb{C}$$

→ Properties of the Pauli matrices:

$$[\sigma_k, \sigma_l] = 2i \sum_{m=1}^3 \epsilon_{klm} \sigma_m \quad \epsilon_{123} = 1 \quad (\text{commutation relation}) \quad (a)$$

$$\{\sigma_k, \sigma_l\} = \sigma_k \sigma_l + \sigma_l \sigma_k = 2 \delta_{kl} \mathbb{1} \quad (\text{anticommutation relation}) \quad (b)$$

↑ "Clifford algebra"
(tracelessness)

$$\text{Tr}(\sigma_k) = 0, \quad k=1,2,3$$

$$\sigma_1 \sigma_2 \sigma_3 = i \mathbb{1}$$

$$\det(\sigma_k) = -1, \quad k=1,2,3 \quad \Rightarrow \text{Pauli matrices have eigenvalues } \{+1, -1\}.$$

$$\sigma_k^* = \sigma_k \quad (\text{Hermiticity})$$

$$\hookrightarrow (a), (b) \Rightarrow \sigma_i \sigma_j = \delta_{ij} \mathbb{1} + i \sum_{k=1}^3 \epsilon_{ijk} \sigma_k$$

→ We have $\sigma_L^2 = \sigma_L \sigma_L = \frac{1}{2} \{ \sigma_L, \sigma_L \} = \mathbb{1}$ ($L=1,2,3$)

$$\Rightarrow \text{Det}(\sigma_L^2) = 1, \text{Tr}[\sigma_L^2] = 2$$

So let a, b be the two eigenvalues of σ_L ($L=1,2,3$), then we have

$$\text{Tr}[\sigma_L] = a+b = 0, \text{Det}(\sigma_L) = a \cdot b = -1, \text{Tr}[\sigma_L^2] = a^2 + b^2 = 2, \text{Det}(\sigma_L^2) = a^2 b^2 = 1$$

$$\Rightarrow a, b = \pm 1$$

The Pauli matrices have the eigenvalues ± 1 .

→ Representation of a density matrix: $S = \frac{1}{2} (\mathbb{1} + \vec{n} \vec{\sigma})$, $\vec{n} \in \mathbb{R}^3$

↳ We automatically have $\text{Tr}(S) = 1$ and $S^\dagger = S$ for $\vec{n} \in \mathbb{R}^3$. We still need to consider the consequences of positivity of S on the possible choices for \vec{n} .

$$S = \frac{1}{2} \begin{pmatrix} 1+u_3 & u_1-iu_2 \\ u_1+iu_2 & 1-u_3 \end{pmatrix},$$

$\text{Tr}(S) = 1 = \text{sum of eigenvalues}, \text{Det}(S) = \frac{1}{4} (1-\vec{n}^2) = \text{product of eigenvalues, which must be} \geq$

$$\Rightarrow \vec{n}^2 \leq 1 \quad \text{and eigenvalues are} \quad S_{1,2} = \frac{1}{2} (1 \pm \sqrt{1-\vec{n}^2})$$

General form of a density matrix: $S = \frac{1}{2} (\mathbb{1} + \vec{n} \vec{\sigma})$, $\vec{n} \in \mathbb{R}^3$ with $|\vec{n}| \leq 1$.

↳ Expectation value of an observable $A = a_0 \mathbb{1} + \vec{a} \vec{\sigma}$, $a_{0,1,2,3} \in \mathbb{R}$:

$$\langle a_0 \mathbb{1} + \vec{a} \vec{\sigma} \rangle = \text{Tr} \left(\frac{1}{2} (\mathbb{1} + \vec{n} \vec{\sigma}) (a_0 \mathbb{1} + \vec{a} \vec{\sigma}) \right) = \text{Tr} \left(\frac{a_0}{2} \mathbb{1} + \frac{a_0}{2} \vec{n} \vec{\sigma} + \frac{1}{2} \vec{a} \vec{\sigma} + \frac{1}{2} (\vec{n} \vec{\sigma})(\vec{a} \vec{\sigma}) \right)$$

$$= a_0 + \vec{n} \vec{a}$$

The set of all possible states in a 2-dim Hilbert space can be represented as the points $\vec{n} \in \mathbb{R}^3$ of the unit sphere, i.e. $|\vec{n}| \leq 1$. ("Bloch Sphere")

Pure state: One of the eigenvalues is 1, the other zero $\Rightarrow \text{Det}(S) = 0 \Rightarrow |\vec{n}| = 1$ (surface)

↳ $S = |X_{\vec{n}} \times X_{\vec{n}}|$ where $|X_{\vec{n}}\rangle$ is the eigenstate to S with eigenvalue 1

$$\text{Representation in } U_2: \quad S = \frac{1}{2} \begin{pmatrix} 1+u_3 & u_1-iu_2 \\ u_1+iu_2 & 1-u_3 \end{pmatrix} = X_{\vec{n}}^- X_{\vec{n}}^+ \quad \text{solid angle: } \vec{n} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{pmatrix}$$

$$\text{for } X_{\vec{n}}^- = \begin{cases} \frac{1}{\sqrt{2(1+u_3)}} \begin{pmatrix} 1+u_3 \\ u_1-iu_2 \end{pmatrix}, & u_3 \neq -1 \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & u_3 = -1 \end{cases}$$

Maximal Mixing: Both eigenvalues are $\frac{1}{2} \Rightarrow \text{Det}(S) = \frac{1}{4} \Rightarrow \vec{n} = (0,0,0)$ (center)