

05/14/2017 ①

## 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 system 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**:

$$q = (q_1, \dots, q_f)$$

→ generalized coordinates

with the canonical coordinates  $q$  and  $p$  in the systems phase space:

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

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

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

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

(iii) Is particle in region  $B \subset \mathbb{R}^6$  (Yes/No)?  $\Rightarrow C_B(\vec{x}, \vec{p}) = \begin{cases} 1, & (\vec{x}, \vec{p}) \in B \\ 0, & (\vec{x}, \vec{p}) \notin B \end{cases}$

The set of all possible values in measurements of observable  $A$  is the set of values  $A(q, p)$  can take 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  $(q_0, p_0)$ .

05/14/2017 (2)

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

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

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

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

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

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

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

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

The state of one single particle is described by

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

↑ norm  
joule kelvin

with  $\int d^3\vec{x} d^3\vec{p} g(\vec{x}, \vec{p}) = 1$

→ 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  $c_{1,2} \in \mathbb{R}$  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.

05/14/2017 (3)

→ 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

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

time-dependent observable

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 (\*) by a change of variables:

$$\begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \rightarrow \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q(t, q_0, p_0) \\ p(t, q_0, p_0) \end{pmatrix}$$

$$\Leftrightarrow \begin{aligned} q_0 &= q_0(t, q, p) && (\text{Inverse exists at least} \\ p_0 &= p_0(t, q, p) && \text{for some time } t > 0.) \end{aligned}$$

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.

An important aspect in the change of variables is **unitarity** which here is connected to the fact that the work 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  $\delta t > 0$ :

$$\Rightarrow q_1 = q(\delta t) = q_0 + \frac{\partial H}{\partial p} \Big|_{t_0} \delta t, \quad p_1 = p(\delta t) = p_0 - \frac{\partial H}{\partial q} \Big|_{t_0} \delta t$$

$$\Rightarrow \text{Det} \left( \frac{dq_1 dp_1}{dq_0 dp_0} \right) = \text{Det} \begin{pmatrix} 1 + \frac{\partial^2 H}{\partial q \partial p} \Big|_{t_0} \delta t & \frac{\partial^2 H}{\partial p^2} \Big|_{t_0} \delta t \\ -\frac{\partial^2 H}{\partial q^2} \Big|_{t_0} \delta t & 1 - \frac{\partial^2 H}{\partial q \partial p} \Big|_{t_0} \delta t \end{pmatrix} = 1 + O(\delta t^2) = 1$$

$|_{t_0}$ : fact of  $q_0, p_0$

because valid at any time  $t$

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

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

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

05/14/2017 (4)

## 4.2. States in Quantum Theory

- For simplicity we consider in the following only systems for which the Hilbert space  $\mathcal{X}$  has  $m$  dimensions,  $m \in \mathbb{N}$ . 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  $\mathcal{X}$  form the operator algebra  $L(\mathcal{X})$  and the Hermitian elements of  $L(\mathcal{X})$  are the observables. Two observables  $A, B \in L(\mathcal{X})$  do in general not commute, i.e. it is possible that  $[A, B] \neq 0$ .

The set of measurable values of an observable  $A \in L(\mathcal{X})$  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 (CONB) of the Hilbert space  $\mathcal{X}$ .

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

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

↳ Form of projectors:  $A|u_\alpha\rangle = a_\alpha|u_\alpha\rangle$ ,  $\langle u_\alpha|u_\alpha\rangle = 1 \Rightarrow P_\alpha = |u_\alpha\rangle\langle u_\alpha|$

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

$P_\alpha$  is a projection operator, so  $P_\alpha = P_\alpha^*P_\alpha = P_\alpha^2 = P_\alpha^+$ .

We now generalize  
the notion "state"

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

(a) Linearity:  $\omega(c_1A_1 + c_2A_2) = c_1\omega(A_1) + c_2\omega(A_2)$ , 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  $\omega$ .

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  $a_\alpha$  in a measurement of observable A when the system is in state  $\omega$ . This is consistent with

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

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

## Different types of States :

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

(2) **Mixed state**: Let  $ω_1, ω_2, \dots, ω_r$  be pure states (related to  $|ψ_1\rangle, \dots, |ψ_r\rangle$ ) and  $0 < p_1, p_2, \dots, p_r < 1$  with  $\sum_{i=1}^r p_i = 1$ ,  $r > 1$ , then

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

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

There is no state  $|ψ\rangle \in \mathcal{X}$ , for which we have  $\omega(A) = \langle ψ|Aψ\rangle$  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  $\{|φ_1\rangle, \dots, |φ_m\rangle\}$  ( $\dim(\mathcal{X}) = m$ ) of  $\mathcal{X}$ . The operation of any operator  $A \in L(\mathcal{X})$  can be written in terms of the matrix elements  $A_{jk} := \langle φ_j|Aφ_k\rangle$ .

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Due to linearity (point (a))  $\omega(A)$  can be written as  $\omega(A) = \sum_{lk} S_{lk} A_{lk}$ .

We can interpret the  $S_{lk}$  as matrix elements  $S_{lk} = \langle \psi_l | S | \psi_k \rangle$  of the abstract operator  $S$ , which fully characterizes the state  $\omega$ . What are the properties of  $S$ ?

$$\hookrightarrow \omega(A) = \sum_{l=1}^m \sum_{k=1}^m \langle \psi_k | S | \psi_l \rangle \psi_l | A | \psi_k \rangle$$

↑ trace ("Spur")

Completeness

$$= \sum_{l=1}^m \langle \psi_l | S A | \psi_l \rangle =: \text{Tr}(S A)$$

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

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

$$\begin{aligned} \langle \psi | S | \psi \rangle &= \sum_{l=1}^m \langle \psi | \psi_l \rangle \psi_l | S | \psi \rangle = \sum_{l=1}^m \langle \psi_l | S | \psi \rangle \psi_l | \psi \rangle = \omega(A) \\ &= \omega(A^\dagger A) \stackrel{(b)}{\geq} 0 \quad \text{for all } |\psi\rangle \in \mathcal{X}, \text{ so } S \text{ is a positive operator.} \end{aligned}$$

$\hookrightarrow$  For positive operators the following statements are equivalent:

1.)  $\langle \psi | S | \psi \rangle \geq 0$  for all  $|\psi\rangle \in \mathcal{X}$

2.)  $S$  is Hermitian and all its eigenvalues are  $\geq 0$

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  $\omega$ . Property (c) will come below.

05/07/2016 (6)

Proof in circle:

1.  $\Rightarrow$  2. Let  $|4_u\rangle$  and  $|4_e\rangle$  be two normalized and orthogonal states .

$$\Rightarrow \langle 4_u + 4_e | S(4_u + 4_e) \rangle = \underbrace{s_{uu}}_{\geq 0} + \underbrace{s_{ee}}_{\geq 0} + \underbrace{s_{ue} + s_{eu}}_{\in \mathbb{C}} \geq 0 \Rightarrow \text{Im}(s_{ue} + s_{eu}) = 0$$

$$\langle 4_u + i4_e | S(4_u + i4_e) \rangle = s_{uu} + s_{ee} + i s_{ue} - i s_{eu} \geq 0 \Rightarrow \text{Re}(s_{ue} - s_{eu}) = 0$$

$$\Rightarrow s_{ue} = s_{eu}^* \Rightarrow s = s^+ \quad (\text{since we can run } |4_u\rangle \text{ and } |4_e\rangle \text{ through a CONS})$$

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  $|4\rangle \in \mathcal{X}$  we have  $\langle 4 | s^+ \rangle = \langle 4 | A^\dagger A^+ \rangle = \langle A^+ A | 4 \rangle \geq 0$

□

↳ Let  $\{|x_1\rangle, \dots, |x_n\rangle\}$  be a CONS of eigenstates of  $s$  with eigenvalues  $s_k \geq 0$

Let  $\{|x_1\rangle, \dots, |x_n\rangle\}$  be a CONB of eigenstates of  $S$  with eigenvalues  $s_k \geq 0$

$$\Rightarrow \omega(\mathbb{I}) = \text{Tr}(S) = 1 \Rightarrow \sum_{k=1}^n s_k = 1$$

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  $A \in L(\mathcal{H})$  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  $S^2 \neq S$ .

This is consistent with

$$\omega(A) = \text{Tr}(SA) = \sum_{k=1}^n \langle x_k | S A | x_k \rangle = \sum_{k=1}^n s_k \underbrace{\langle x_k | A | x_k \rangle}_{\text{Quantum mechanical expectation value}}$$

Classical statistical probability  
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  $S_\psi = |\psi\rangle \langle \psi|$  represents a system being with probability 1 in the (normalized) state  $|\psi\rangle \in \mathcal{H}$ . Then  $S_\psi$  is a projector with  $S_\psi^2 = S_\psi$  and we have

$$\omega_\psi(A) = \sum_{k=1}^n \langle x_k | |\psi\rangle \langle \psi| A | x_k \rangle = \sum_{k=1}^n \langle \psi | A | x_k \rangle \langle x_k | \psi \rangle = \langle \psi | A | \psi \rangle$$

as it should be.

Example:

(1) State of maximal mixing

Let be  $\dim(\mathcal{X}) = n$ , then  $\mathbf{g} = \frac{1}{n} \mathbf{1}$  has only the eigenvalue  $\frac{1}{n}$  where all states are eigenstates. For any given CONR this state represents a statistical mixture where each state of the CONR 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  $T$ :

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

Let  $\{|e_1\rangle, \dots, |e_n\rangle\}$  be a CONR of energy eigenstates with  $H|e_i\rangle = E_i|e_i\rangle$ ,  $i=1, \dots, n$ , then the spectral representation of  $\mathbf{g}$  has the form

$$\mathbf{g} = \frac{1}{Z} \sum_{i=1}^n e^{-E_i/kT} |\psi_i\rangle \langle \psi_i|, \quad Z = \sum_{i=1}^n e^{-E_i/kT}$$

(3) Pure vs. mixed state

(part A)

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

Let  $|4_1\rangle$  and  $|4_2\rangle$  be two orthonormal states.

(a) pure state  $|4\rangle = \frac{1}{\sqrt{2}}(|4_1\rangle + |4_2\rangle)$

$$\rightarrow S_4 = |4 \times 4| = \frac{1}{2} |4_1 \times 4_1| + \frac{1}{2} |4_2 \times 4_2| + \underbrace{\frac{1}{2} (|4_1 \times 4_2| + |4_2 \times 4_1|)}_{\substack{\text{"off-diagonal terms"} \\ \text{"interference term"}}}$$

(b) mixed state : 50%  $|4_1\rangle$  and 50%  $|4_2\rangle$

$$\rightarrow S_{50\%} = \frac{1}{2} |4_1 \times 4_1| + \frac{1}{2} |4_2 \times 4_2|$$

$\rightarrow$  general uncertainty relation for arbitrary states

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

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

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

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  $S_p$  and the mixed state  $S_{\text{mixed}}$  will always give the value  $\alpha$  in measurements of A, with  $\Delta_w A = 0$ .

It is possible to construct infinitely many such different states that always yield the same value  $\alpha$  in a measurement of A, with  $\Delta_w A = 0$ .

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

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

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  $\Delta_w A = 0$  if and only if  $A_S = gA = \alpha g$  where  $\alpha$  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):

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  $\rho$  it is always possible to find an observable  $A$  such that  $[A, \rho] \neq 0$ .

Proof: Take observable  $B = B^+$  with  $\omega(B^2) = 0$ . Let be  $\rho = \sum_{k=1}^n s_k |x_k x_k|$ ,  $\{|x_k\rangle\}$  is CONB.

$$\Leftrightarrow 0 = \text{Tr}(\rho B^2) = \sum_{k=1}^n s_k \langle x_k | B^2 x_k \rangle = \underbrace{\sum_{k=1}^n s_k}_{\geq 0} \underbrace{\langle B x_k | B x_k \rangle}_{\geq 0}$$

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

$$\Leftrightarrow \langle x_l | B | x_k \rangle = \langle x_k | B | x_k \rangle = 0, l=1, \dots, n \text{ für alle } s_k \neq 0 \Leftrightarrow B\rho = \rho B = 0$$

↳ Take  $B = A - \omega(A)$  then  $B\rho = \rho B = 0 \Leftrightarrow A\rho = \rho A = \omega(A)\rho$   $\blacksquare$

→ 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:  $A = \sum_{\alpha=1}^m a_\alpha P_\alpha$ ,  $a_\alpha + a_\beta$  for  $\alpha \neq \beta$ ,  $P_\alpha$ : project on eigenspace to eigenvalue  $a_\alpha$

State prior to measurement :  $S$

State after the measurement of the value  $a_\alpha$  :  $S' = \frac{P_\alpha S P_\alpha}{\text{Tr}(P_\alpha S P_\alpha)}$

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

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

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

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

Educational exercises :

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

05/11/2016 ①

### 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")

- ② Time dependence contained in the states
- ② 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:  $|\psi_S(t)\rangle = U_S(t) |\psi_S(0)\rangle$ ,  $U_S(t) = \underbrace{\exp(-iH_S t/\hbar)}$

unitary time-evolution operator:  $U_S^+(t) = U_S^{-1}(t)$   
 $= \exp(iH_S t/\hbar)$

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

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

Time evolution of the density operator:

$$\rho_S(t) = U_S(t) \rho_S(0) U_S^+(t)$$

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

Time evolution of the density operator :  $\rho_s(t) = U_s(t) \rho_s(0) U_s^*(t)$

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

Derivation:  $\frac{d}{dt} U_s(t) = -\frac{i}{\hbar} H U_s(t) = -\frac{i}{\hbar} U_s(t) , \frac{d}{dt} U_s^*(t) = \frac{i}{\hbar} H U_s^*(t) = \frac{i}{\hbar} U_s^*(t) H$   
 $\Rightarrow \frac{d}{dt} \rho_s(t) = -\frac{i}{\hbar} (H \rho_s(t) - \rho_s(t) H)$

Observables: time-independent Hermitian operators in  $L(\mathbb{X})$

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

→ 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

$$\omega_t(A) = \text{Tr}(\rho_s(t) A_s) = \text{Tr}(U_s(t) \rho_s(0) U_s^*(t) A_s)$$

$$= \text{Tr}(\rho_s(0) U_s^*(t) A_s U_s(t))$$

$$\omega_t(A) = \text{Tr}(\rho_H A_H(t)) \quad \text{with} \quad \rho_H = \rho_s(0), \quad A_H(t) = U_s^*(t) A_s U_s(t)$$

time-independent state  
time-dependent observable

$$\Rightarrow U_s^*(t) A_H(0) U_s(t)$$

05/11/2016 (2)

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

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

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  $V(r)$

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

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

$$[X_n(t), P_n(t)] = [U_s^\dagger(t) X_s U_s(t), U_s^\dagger(t) P_s U_s(t)] = \underbrace{U_s^\dagger(t)}_{it\hbar\mathbb{1}} [X_s, P_s] U_s(t)$$

$$= \frac{i}{\hbar} \left[ -\frac{m}{2\omega_0}, X_h(t) \right]$$

$$[X_h(t), P_h(t)] = [U_s^+(t) X_s U_s(t), U_s^+(t) P_s U_s(t)] = U_s^+(t) \underbrace{[X_s, P_s]}_{i\hbar \mathbb{1}} U_s(t)$$

$$= i\hbar \mathbb{1}$$

$$\Rightarrow [P^2, X] = P[P, X] + [P, X]P = -2i\hbar P$$

$$\Rightarrow \dot{X}_h(t) = \frac{\dot{P}_h(t)}{m}$$

$$\hookrightarrow \dot{P}_h(t) = \frac{i}{\hbar} [H_h(t), P_h(t)] = \frac{i}{\hbar} [V(X_h(t)), P_h(t)]$$

$$[V(X), P] = i\hbar V'(X)$$

$$\dot{P}_h(t) = -V'(X_h(t))$$

## 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 CONS  $\{|1\rangle, |2\rangle\}$  of  $\mathcal{X}$ :  $\langle 1|1\rangle = \langle 2|2\rangle = 1$ ,  $\langle 1|2\rangle = 0$ , (orthonormality)

$$|1\rangle\langle 1| + |2\rangle\langle 2| = \mathbb{1} = \mathbb{1}_{2 \times 2}$$

(completeness)

All  $|4\rangle \in \mathcal{X}$  are a linear combination of  $|1\rangle$  and  $|2\rangle$ :  $|4\rangle = |1\rangle \underbrace{\langle 1|4\rangle}_{c_1} + |2\rangle \underbrace{\langle 2|4\rangle}_{c_2} = c_1|1\rangle + c_2|2\rangle$ ,  $c_{1,2} \in \mathbb{C}$

Scalar product:  $\langle x|4\rangle = b_1^* c_1 + b_2^* c_2$  for  $|x\rangle = b_1|1\rangle + b_2|2\rangle$

↳ Every state can be unique written as 2-dim complex vector:  $|4\rangle \in \mathcal{X} \Leftrightarrow \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, c_{1,2} \in \mathbb{C}$

with the scalar product:  $\langle x|4\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}^* \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = (b_1^*, b_2^*) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = b_1^* c_1 + b_2^* c_2$

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

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

$$A = A_{11}|1\rangle\langle 1| + A_{21}|1\rangle\langle 2| + A_{12}|2\rangle\langle 1| + A_{22}|2\rangle\langle 2|$$

$$A = A_{\uparrow\uparrow} | \uparrow\uparrow \rangle\langle \uparrow\uparrow | + A_{\downarrow\downarrow} | \downarrow\downarrow \rangle\langle \downarrow\downarrow | + A_{\uparrow\downarrow} | \uparrow\downarrow \rangle\langle \uparrow\downarrow | + A_{\downarrow\uparrow} | \downarrow\uparrow \rangle\langle \downarrow\uparrow |$$

which also has the matrix representation  
with respect to the CNOT f  $| \uparrow\uparrow \rangle, | \downarrow\downarrow \rangle \}$

$$A = \begin{pmatrix} A_{\uparrow\uparrow} & A_{\uparrow\downarrow} \\ A_{\downarrow\uparrow} & A_{\downarrow\downarrow} \end{pmatrix}, \quad A_{\mu\nu} \in \mathbb{C} \quad \left. \begin{array}{l} \text{arbitrary complex} \\ 2 \times 2 \text{ matrix} \end{array} \right\}$$

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

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

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

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

→ 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"

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

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

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

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

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

05/11/2016 (4)

$$\rightarrow \text{We have } \sigma_l^2 = \sigma_l \sigma_k = \frac{1}{2} \{ \sigma_l, \sigma_k \} = 1 \quad (l=1,2,3)$$

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

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

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

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

The Pauli matrices have the eigenvalues  $\pm 1$ .

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

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

$$\rho = \frac{1}{2} \begin{pmatrix} 1+n_3 & n_1-i n_2 \\ n_1+i n_2 & 1-n_3 \end{pmatrix},$$

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

$$\Rightarrow \vec{n}^2 \leq 1 \text{ and eigenvalues are } \rho_{1,2} = \frac{1}{2} (1 \pm |\vec{n}|)$$

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

$\hookrightarrow$  Expectation value of an observable  $A = a_0 \mathbb{1} + a_1 \vec{\sigma}$ ,  $a_0, a_1 \in \mathbb{R}$ :

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

↳ Expectation value of an observable  $A = a_0\mathbb{1} + \vec{a}\vec{\sigma}$ ,  $a_0, a_1, a_2 \in \mathbb{R}$ :

$$\begin{aligned}\langle a_0\mathbb{1} + \vec{a}\vec{\sigma} \rangle &= \text{Tr}\left(\frac{1}{2}(\mathbb{1} + \vec{u}\vec{\sigma})(a_0\mathbb{1} + \vec{a}\vec{\sigma})\right) = \text{Tr}\left(\frac{a_0}{2}\mathbb{1} + \frac{a_0}{2}\vec{u}\vec{\sigma} + \frac{1}{2}\vec{a}\vec{\sigma} + \frac{1}{2}(\vec{u}\vec{\sigma})(\vec{a}\vec{\sigma})\right) \\ &= a_0 + \vec{u}\vec{a}\end{aligned}$$

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

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

↳  $\rho = |\chi_{\vec{u}}\rangle\langle\chi_{\vec{u}}|$  where  $|\chi_{\vec{u}}\rangle$  is the eigenstate to  $\rho$  with eigenvalue 1

Representation in  $U_2$ :  $\rho = \frac{1}{2} \begin{pmatrix} 1+u_3 & u_1+iu_2 \\ u_1-iu_2 & 1-u_3 \end{pmatrix} = |\chi_{\vec{u}}\rangle\langle\chi_{\vec{u}}|$  solid angles:  $\vec{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} \sin\theta \cos\varphi \\ \sin\theta \sin\varphi \\ \cos\theta \end{pmatrix}$

for  $|\chi_{\vec{u}}\rangle = \begin{cases} \frac{1}{\sqrt{2(1+u_3)}} \begin{pmatrix} 1+u_3 \\ u_1+iu_2 \end{pmatrix}, & u_3 \neq -1 \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & u_3 = -1 \end{cases}$

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