Statistical ensemble (mixture), density operator

quantum system prepared in one out of N states

$|\psi_1\rangle, |\psi_2\rangle, \dots |\psi_N\rangle$ with prob.

$p_1, p_2, \dots, p_N$

forms a statistical ensemble

$$\mathcal{E} = \{p_i, |\psi_i\rangle\}_{i=1,\dots,N}$$

- $p_i \geq 0$; $\sum_i p_i = 1$
- note: $|\psi_i\rangle$ not necessarily orthogonal!

Examples:

1) pure state / trivial ensemble:

$$\mathcal{E}_1 = \{ 1, |\psi\rangle \}$$

2) totally mixed ensemble:

$$\mathcal{E}_2 = \left\{ \frac{1}{d}, |\varphi_i\rangle \right\}_{i=1,\dots,d}$$

where $|\varphi_1\rangle, \dots, |\varphi_d\rangle$ ONB of $\mathcal{H}$

3) ensemble originating from ideal measurement of observable $A = \sum_{l=1}^{N} a_l P_l$

$$|\psi\rangle \begin{array}{l} \xrightarrow{p_1} |\psi_1\rangle \\ \xrightarrow{p_2} |\psi_2\rangle \\ \quad\vdots \\ \xrightarrow{p_N} |\psi_N\rangle \end{array}$$

where $p_l = \langle \psi | P_l | \psi \rangle$, $|\psi_l\rangle = \frac{1}{\sqrt{p_l}} P_l |\psi\rangle$

i. e. :

$$\{1, |\psi\rangle\} \xrightarrow[\text{measurement of } A]{\text{ideal}} \{p_\ell, |\psi_\ell\rangle\}_{\ell=1,\dots,N}$$

Density operator

- statist. ensemble $\mathcal{E} = \{p_\ell, |\psi_\ell\rangle\}$
- obervable $A = \sum_i a_i P_i$

$\rightarrow$ expectation value of A in $\mathcal{E}$:

$$\langle A \rangle_{\mathcal{E}} = \sum_\ell p_\ell \langle A \rangle_{\psi_\ell}$$

$$= \sum_\ell p_\ell \langle \psi_\ell | A | \psi_\ell \rangle$$

$$= \sum_\ell p_\ell \, tr\left(|\psi_\ell\rangle\langle\psi_\ell| A \right)$$

$$= tr\Big(\underbrace{\sum_\ell p_\ell |\psi_\ell\rangle\langle\psi_\ell|}_{= \rho_{\mathcal{E}}} \; A \Big)$$

density operator for stat. ens. $\mathcal{E}$:

$$\rho_{\mathcal{E}} := \sum_{l=1}^{N} w_l \, |\psi_l\rangle\langle\psi_l|$$

$$\rightarrow \quad \langle A \rangle_{\mathcal{E}} = tr(\rho_{\mathcal{E}} A) \quad .$$

general properties:

- $\rho_{\mathcal{E}} \geq 0$ (i.e.: $\forall \psi$: $\langle\psi|\rho_{\mathcal{E}}|\psi\rangle \geq 0$;

  equiv.: • $\rho_{\mathcal{E}} = \rho_{\mathcal{E}}^{\dagger}$

  • eigenval. $\lambda_l \geq 0$)

- $tr \, \rho_{\mathcal{E}} = 1$

Note:

(a) all we know about a statist. ensemble $\mathcal{E}$ we know from measurement outcomes!

(b) measurement outcomes $\hat{=}$ expectation values are determined by density operator ϱ_ε

(a), (b) $\longrightarrow$ two ensembles ε and ε' with identical dens. op.s $\varrho_\varepsilon \overset{!}{=} \varrho_{\varepsilon'}$ are physically indistinguishable !

Example:

spin $1/2$; $\mathcal{H} = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}$

$$\varepsilon = \{ (\tfrac{1}{2}, |\uparrow\rangle), (\tfrac{1}{2}, |\downarrow\rangle) \}$$

$$\varepsilon' = \{ (1/2, |x+\rangle), (1/2, |x-\rangle) \}$$

$$|x\pm\rangle = (|\uparrow\rangle \pm |\downarrow\rangle) / \sqrt{2}$$

$$\rightarrow \quad \rho_\varepsilon = \frac{1}{2}\mathbb{1}_2 = \rho_{\varepsilon'}$$

i.e. „$\varepsilon \overset{!}{=} \varepsilon'$"

<u>Thm:</u>

ρ density operator, i.e. $\rho \geq 0$, $\operatorname{tr}\rho = 1$

$\Longleftrightarrow$ $\exists$ stat. ens. ε st. $\rho = \rho_\varepsilon$

(exercise)

<u>Conclusion:</u>

The quantum-statistical state of a quantum system is <u>completely</u> described by a density operator.

$\Rightarrow$: • <u>quantum state</u> $\hat{=}$ <u>density operator ρ</u>

($\rho \geq 0$, $\operatorname{tr}\rho = 1$)

• <u>pure state</u> $\hat{=}$ <u>rank 1</u> density operator:

$\rho \overset{!}{=} |\psi\rangle\langle\psi|$ $(\hat{=} \; |\psi\rangle)$

• <u>mixed</u> state $\hat{=}$ $\neg$ pure state

Examples:

(a) totally mixed state:

$$\rho = \frac{1}{d}\,\mathbb{1} \quad \left(= \sum_{l=1}^{d} \frac{1}{d} |\varphi_l\rangle\langle\varphi_l|\right)$$

(b) mixed state generated by ideal measurement of observable

$$A = \sum_{l=1}^{N} a_l \, P_l$$

on pure state $|\psi\rangle$:

$$\begin{array}{ccc} \{1, |\psi\rangle\} & \longrightarrow & \{\mu_l, |\psi_l\rangle\}_{l=1,\dots,N} \\ \downarrow & & \downarrow \\ \rho = |\psi\rangle\langle\psi| & \longrightarrow & \rho' = \sum_l \mu_l \, |\psi_l\rangle\langle\psi_l| \end{array}$$

with $\mu_l = \langle\psi|P_l|\psi\rangle$, $|\psi_l\rangle = \frac{1}{\sqrt{\mu_l}} P_l|\psi\rangle$:

$$\rho' = \sum_l P_l|\psi\rangle\langle\psi|P_l = \underline{\sum_l P_l \, \rho \, P_l}$$

holds for general initial state!

$$\varrho \xrightarrow[A \text{ measurement}]{} \varrho' = \sum_\ell P_\ell \varrho P_\ell .$$

Postulates reformulated for general states:

(P1') quantum state = density operator ϱ on $\mathcal{H}$,

$$\varrho \geq 0 , \quad \operatorname{tr} \varrho = 1$$

(P2') Measurement

observable $\hat{=}$ hermitian operator

$$A = \sum_\ell a_\ell P_\ell$$

$\rightarrow$ expectation value of A in state ϱ:

$$\langle A \rangle_\varrho = \operatorname{tr} \varrho A$$

$\rightarrow$ state immediately after ideal measurement:

$$\varrho' = \sum_\ell P_\ell \varrho P_\ell$$

(P3') <u>Dynamics</u>

$$\rho(t) = U_t \, \rho(0) \, U_t^{\dagger}$$

$$\uparrow \; U_t = e^{-iHt}$$

equivalently:

$$\dot{\rho}(t) = -i \, [H, \rho(t)]$$

Quantum mechanics of joint systems

(needed for e.g. • qubit register
• open quantum system)

AB:

A: $\mathcal{H}_A$

ONB

$|\varphi_1\rangle, \dots, |\varphi_n\rangle$

B: $\mathcal{H}_B$

ONB

$|\chi_1\rangle, \dots, |\chi_m\rangle$

$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$,

<u>ONB</u> : $\{ |\varphi_i \, \chi_j\rangle \}_{\substack{i=1,\dots,n \\ j=1,\dots,m}}$!

- $\mathcal{H}_A \otimes \mathcal{H}_B$: "<u>tensorproduct</u> of $\mathcal{H}_A$ and $\mathcal{H}_B$"
- $|\varphi_i \chi_j\rangle = |\varphi_i\rangle|\chi_j\rangle = |\varphi_i\rangle \otimes |\chi_j\rangle = \varphi_i \otimes \chi_j$

  <u>ONB</u> !
- $\dim \mathcal{H}_A \otimes \mathcal{H}_B = \dim \mathcal{H}_A \cdot \dim \mathcal{H}_B$
- general $\psi_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$:

$$\psi_{AB} = \sum_{ij} a_{ij} \, \varphi_i \otimes \chi_j$$

- <u>tensorproduct of vectors</u> :

$$\psi = \sum_i \alpha_i \, \varphi_i \in \mathcal{H}_A$$

$$\vartheta = \sum_j \beta_j \, \chi_j \in \mathcal{H}_B$$

$$\longrightarrow \quad \psi \otimes \vartheta = \sum_{ij} \alpha_i \beta_j \, \varphi_i \otimes \chi_j$$

- <u>tensorproduct of operators</u> :

$$V \in \mathcal{L}(\mathcal{H}_A), \quad W \in \mathcal{L}(\mathcal{H}_B)$$

$$\longrightarrow \quad (V \otimes W)(\varphi_i \otimes \chi_j) := (V\varphi_i) \otimes (W\chi_j),$$

and by linearity for general $\psi_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$

Entanglement:

Pure state $|\psi_{AB}\rangle$ separable iff

$$|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$$

for suitable $|\psi_A\rangle \in \mathcal{H}_A$, $|\psi_B\rangle \in \mathcal{H}_B$,

otherwise $|\psi_{AB}\rangle$ entangled.

Partial trace and reduced density operator

Partial trace:

- $\operatorname{tr}_B(\sigma_A \otimes \sigma_B) := (\operatorname{tr}\sigma_B)\,\sigma_A \quad \in \mathcal{L}(\mathcal{H}_A)$
- $\operatorname{tr}_A(\sigma_A \otimes \sigma_B) := (\operatorname{tr}\sigma_A)\,\sigma_B \quad \in \mathcal{L}(\mathcal{H}_B)$

and by linearity for general $\sigma_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$

thus:

(i) $\sigma_{AB} = \sum_{ij,lm} a_{ij,lm} |\varphi_i\rangle\langle\varphi_j| \otimes |\chi_l\rangle\langle\chi_m|$

$\longrightarrow \quad tr_B\, \sigma_{AB} = \sum_{ij} \sum_{l} a_{ij,ll} |\varphi_i\rangle\langle\varphi_j|$

$\longrightarrow \quad tr_A\, \sigma_{AB} = \sum_{lm} \sum_{i} a_{ii,lm} |\chi_l\rangle\langle\chi_m|$

(ii) $tr\, \sigma_{AB} = tr_A (tr_B\, \sigma_{AB})$

$= tr_B (tr_A\, \sigma_{AB})$

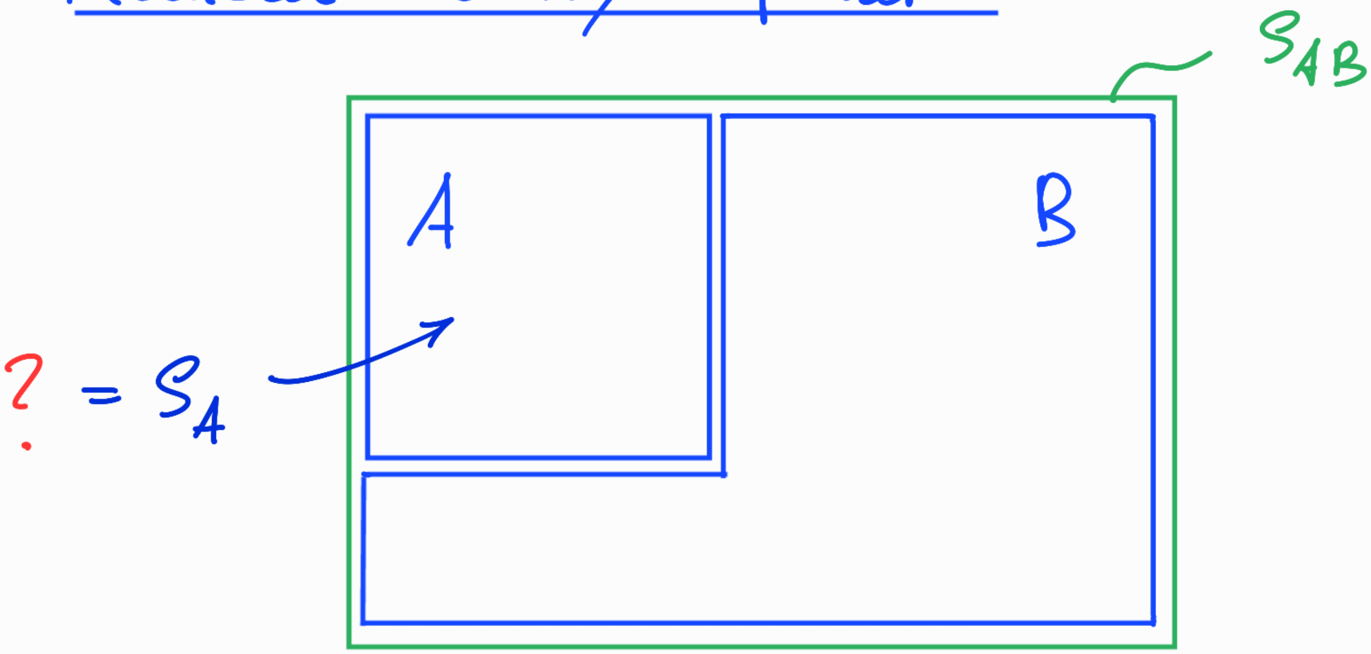
(iii) $tr_B [(V \otimes \mathbb{1}_B)\, \sigma_{AB}] = V\, tr_B\, \sigma_{AB}$

$\Big\lceil$ w.l.o.g. $\sigma_{AB} = \sigma_A \otimes \sigma_B$;

$\rightarrow tr_B (V \otimes \mathbb{1}_B)\, \sigma_{AB} = tr_B (V\sigma_A \otimes \sigma_B)$

$= V\sigma_A\, tr\, \sigma_B = V\, tr_B\, \sigma_{AB}$ $\Big\rfloor$

Reduced density operator



If AB is in state ϱ_{AB}, what is the quantum state of subsystem A ?

Consider A-local observable :

$$\sigma_A \otimes \mathbb{1}_B$$

$$\rightarrow \langle \sigma_A \otimes \mathbb{1}_B \rangle_{\varrho_{AB}} = \mathrm{tr}\, \varrho_{AB} (\sigma_A \otimes \mathbb{1}_B)$$

$$\overset{(iii)}{=} \mathrm{tr}_A\big(\sigma_A \underbrace{\mathrm{tr}_B\, \rho_{AB}}_{\overset{!}{=}\rho_A\,!}\big) \overset{!}{=} \langle \sigma_A \rangle_{\rho_A}$$

$\rightarrow$ the state of A is given by the <u>reduced density operator</u>

$$\rho_A = \mathrm{tr}_B\, \rho_{AB}$$

<u>Example</u>: AB in <u>pure</u> state

$$|\psi_{AB}\rangle = \sum_i \alpha_i\, |\varphi_i\rangle\, |\chi_i\rangle$$

(entangled!)

i.e.

$$\rho_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}| = \sum_{ij} \alpha_i \alpha_j^* \, |\varphi_i\rangle\langle\varphi_j| \otimes |\chi_i\rangle\langle\chi_j|$$

$\rightarrow$

$\rightarrow$ subsystem A in <u>mixed</u> state

$$\rho_A = \mathrm{tr}_B\, \rho_{AB} = \sum_i |\alpha_i|^2 |\varphi_i\rangle\langle\varphi_i|$$

$\rightarrow$ A <u>mixed</u> state can be a <u>reduced</u> <u>pure</u> state of a larger system:

$$|\psi_{AB}\rangle \xrightarrow{\mathrm{tr}_B} \rho_A$$

$\hookrightarrow$ <u>purification</u> of ρ_A

(later more about that ...)