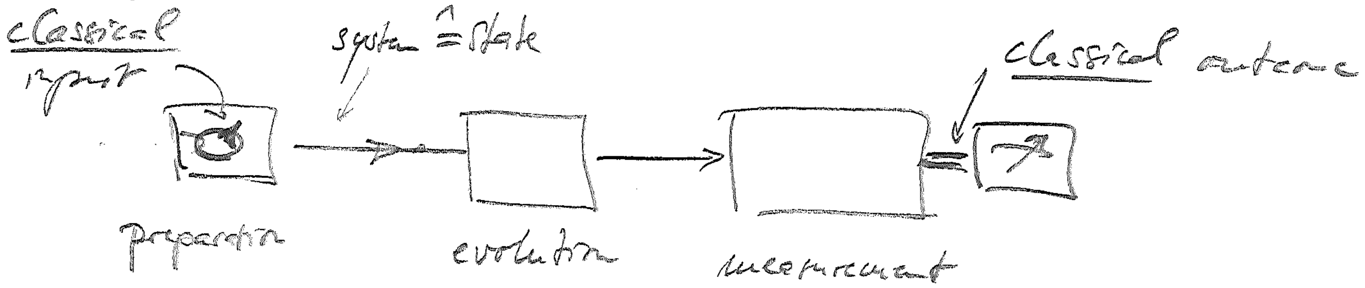
II. The formalism: States, measurements, and evolution

1. Axioms ("pure" version):

- Setup in Q.M.:



- State of the system = description of our knowledge of system (= prediction of outcomes ...)

- States are vectors in Hilbert spaces!

  (More precisely: rays.)

Hilbert space: $\mathcal{H}$ is a Hilbert space iff

i) $\mathcal{H}$ is a vector space over $\mathbb{C}$. We denote vectors by $|v\rangle \in \mathcal{H}$.

ii) $\mathcal{H}$ has a scalar product $\langle v|w\rangle$ s.t.

- $\langle v|v\rangle > 0$ if $|v\rangle \neq 0$

- $\langle v| a_1 w_1 + a_2 w_2\rangle = a_1\langle v|w_1\rangle + a_2\langle v|w_2\rangle$

  for $a_1, a_2 \in \mathbb{C}$.

- $\langle v|w\rangle = \langle w|v\rangle^*$

iii) $\mathcal{H}$ is <u>complete</u> in the norm

$$\|v\| = \sqrt{\langle v|v\rangle}$$

(<u>Note</u>: The property iii) – completeness – is always satisfied in finite dimensions – which we focus on – so we can safely ignore it most of the time)

<u>Ket/bra notation:</u>

$|v\rangle$ denotes vectors ("column vectors"),

$\langle v|$ denotes their duals ("row vectors")

$$\langle v| \cdot |w\rangle \equiv \langle v|w\rangle$$

<u>Basis</u>:

We can expand vectors in an orthonormal basis

$$|e_i\rangle \equiv |i\rangle, \qquad \langle i|j\rangle = \delta_{ij}$$

$$\Rightarrow |v\rangle = \sum_{i=1}^{d} v_i |i\rangle = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix}$$

$$\langle v| = \sum_i v_i^* \langle i| = (v_1^*, \dots, v_d^*)$$

Quantum systems $\longleftrightarrow$ Hilbert space $\mathcal{H}$

State of system $\longrightarrow$ vector $|\psi\rangle \in \mathcal{H}$ with $\||\psi\rangle\| = 1$.

<u>Note</u>: States $|\psi\rangle$ and $c|\psi\rangle$ describe the same state.

Linear operators:

$M : \mathcal{H} \longrightarrow \mathcal{H}$ is linear:

$$M(|v\rangle + \alpha|w\rangle) = M(|v\rangle) + \alpha M(|w\rangle) \quad \text{for } \alpha \in \mathbb{C}.$$

Write $\quad M(|v\rangle) = M|v\rangle.$

Expansion in ONB:

$$M = \left(\sum_i^d |i\rangle\langle i|\right) M \left(\sum_j^d |j\rangle\langle j|\right)$$

$$= \sum_{ij}^d M_{ij}\, |i\rangle\langle j| = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1d} \\ \vdots & & & \\ M_{d1} & \cdots & \cdots & M_{dd} \end{pmatrix}$$

with $\quad M_{ij} = \langle i|M|j\rangle.$

∘ Evolution: unitary transformation $U : \mathcal{H} \to \mathcal{H}$.

$$|\psi\rangle \longmapsto U|\psi\rangle.$$

Unitary: $\quad \underbrace{(U|\psi\rangle)^\dagger}_{=\langle\psi|U^\dagger} \cdot (U|\phi\rangle) = \langle\psi|\phi\rangle$, i.e., angle-preserving.

In basis: $\quad (U^\dagger)_{ij} = U^{*}_{ji}\;;$

Unitarity $\Longleftrightarrow$ $U^\dagger U = \mathbb{1}.$

- Hamiltonians:

Unitary evolution is generated by a Hamiltonian H, $H = H^\dagger$:

Infinitesimal $\mathcal{U} \approx \mathbb{1} + \delta t \cdot K$:

$$\mathbb{1} = \mathcal{U}^\dagger \mathcal{U} = (\mathbb{1} + \delta t K^\dagger)(\mathbb{1} + \delta t K)$$

$$= \mathbb{1} + \delta t \underbrace{(K + K^\dagger)}_{\overset{!}{=} 0} + O(\delta t^2)$$

$\Rightarrow K = -K^\dagger$. With $H = iK$: $H = H^\dagger$.

Unitaries $\leftrightarrow$ evolve with Hamiltonian $H(t)$,

$$\mathcal{U}(t) = e^{iHt} \quad \text{or} \quad \mathcal{U}(t) = \mathcal{T} e^{\int iH(t)dt}.$$

- Measurement:

Observable quantities = $\underbrace{\text{hermitian}}_{\text{i.e. } A = A^\dagger}$ operators A

Eigenvalue decomposition: eigenbasis of A!

$$A = \sum_{n=1}^{d} a_n |n\rangle\langle n| = \sum a_n E_n$$

spectral projector: $|n\rangle\langle n|$, or $\sum' |n\rangle\langle n|$ for degen. eigenvalues)

$\sum'$: n degen.

Measurement of A on state $|\psi\rangle$:

Outcome a_n with probability $|\langle n|\psi\rangle|^2$

or $\langle\psi|E_n|\psi\rangle = \| E_n|\psi\rangle\|^2$.

State after measurement:

$$|\psi_n\rangle = \frac{E_n|\psi\rangle}{\| E_n|\psi\rangle\|}$$

Expectation value (= average meas. outcome):

$$\langle\psi|A|\psi\rangle = \sum a_n \langle\psi|E_n|\psi\rangle.$$

Axioms: • States are vectors $|\psi\rangle \in \mathcal{H}$, $\||\psi\rangle\| = 1$,

with $|\psi\rangle \sim c|\psi\rangle$ the same state (rays).

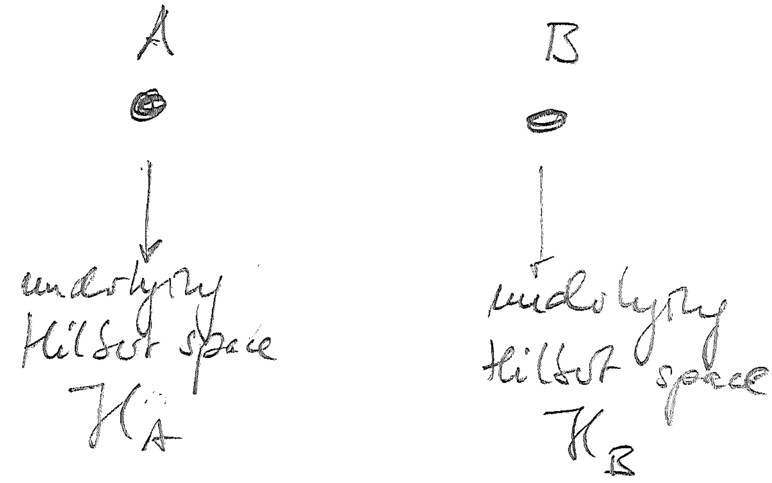
• Evolution $U: |\psi\rangle \mapsto U|\psi\rangle$ is unitary.

• Measurements $A = \sum a_n E_n \leftarrow$ proj. act as

$$|\psi\rangle \mapsto |\psi_n\rangle = \frac{E_n|\psi\rangle}{\|E_n|\psi\rangle\|} \text{ w/ prob. } \|E_n|\psi\rangle\|^2.$$

- Composite systems:

  - We consider a system with two separate parts ("subsystems") A (= Alice) and B (= Bob).



$\Rightarrow$ Joint system: Underlying Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$.

$\rightarrow$ State described by $|\psi\rangle_{AB} \in \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$.

General form of vector in $\mathcal{H}_A \otimes \mathcal{H}_B$?

$$|i\rangle_A \quad \text{ONB of } \mathcal{H}_A, \quad i = 1, \dots, d_A$$

$$|j\rangle_B \quad \text{ONB of } \mathcal{H}_B, \quad j = 1, \dots, d_B.$$

$$\Rightarrow \quad |i\rangle_A \otimes |j\rangle_B = |i\rangle_A |j\rangle_B = |i, j\rangle_{AB} = |ij\rangle_{AB}$$

basis of $\mathcal{H}_A \otimes \mathcal{H}_B$; $\quad i = 1, \dots, d_A; \; j = 1, \dots, d_B$

$|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$:

$$|\psi\rangle = \sum c_{ij}\, |i\rangle_A |j\rangle_B \quad : \quad d_A \times d_B \text{ - dimensional.}$$

$$= (c_{11}, c_{12}, c_{13} \ldots c_{1d_B}, c_{21}, c_{22}, \ldots, c_{d_A d_B})^T.$$

What happens if Alice acts w/ M_A on her system, and Bob with N_B on his?

(Note: M_A, N_B could be unitaries, measurements, meas. projectors E_n, ... — or even the trivial action $N_B = \mathbb{1}_B$ if only Alice acts on her system.)

Total action given by $M_A \otimes N_B$:

$$(M_A \otimes N_B)(|i\rangle_A \otimes |j\rangle_B) = (M_A |i\rangle_A) \otimes (N_B |i\rangle_B)$$

Matrix elements:

$$\langle i_A i_B | M_A \otimes N_B | j_A j_B \rangle = \langle i_A | M_A | j_A \rangle \langle i_B | N_B | j_B \rangle$$

$$\|$$

$$(M_A \otimes N_B)_{(i_A i_B)(j_A j_B)} = (M_A)_{i_A j_A} (N_B)_{i_B j_B}$$

Matrix notation:

$$(\Pi_A \otimes N_B) = \left(\begin{array}{c|c} (\Pi_A)_{11} N_B & (\Pi_A)_{12} N_B \quad \cdots \\ \hline (\Pi_A)_{12} \cdot N_B & \\ \vdots & \ddots \end{array}\right)$$

Examples:

Qubits: $\mathcal{H} = \mathbb{C}^2$; "computational basis" $|0\rangle, |1\rangle$

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad , \quad |\alpha|^2 + |\beta|^2 = 1$$

Observable $$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \underbrace{\overbrace{|0\rangle\langle 0|}^{E_0} - \overbrace{|1\rangle\langle 1|}^{E_1}}_{\text{eigenbasis!}}$$

$\to$ eigenvalues $+1$ w/ eigenvector $|0\rangle$

-1 w/ eigenvector $|1\rangle$

Measurement: $$\frac{E_0|\psi\rangle}{\| E_0|\psi\rangle \|} = |0\rangle \quad \text{w. prob. } \| E_0 |\psi\rangle \|^2 = |\alpha|^2$$

$$\frac{E_1|\psi\rangle}{\| E_1|\psi\rangle \|} = |1\rangle \quad \text{w. prob. } \| E_1 |\psi\rangle \|^2 = |\beta|^2$$

Observable $$X = |0\rangle\langle 1| + |1\rangle\langle 0| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \underbrace{\overbrace{|+\rangle\langle +|}^{E_+} - \overbrace{|-\rangle\langle -|}^{E_-}}_{\text{eigensystem}}$$

with $|\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle)$

Measurement:

$$\frac{E_\pm|\psi\rangle}{\|E_\pm|\psi\rangle\|} = |\pm\rangle \text{ w. prob. } |\langle\pm|(\alpha|0\rangle+\beta|1\rangle)|^2 = \frac{|\alpha\pm\beta|^2}{2}$$

Evolution:

Ham. $Y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$. Evolve for time $\pi/4$ $(\hbar = 1!)$

$$U = e^{-i\pi/4 \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}} \quad . \quad \text{Use } Y^2 = \mathbb{1}$$

$$= \cos(\pi/4)\mathbb{1} - i\sin(\pi/4)Y$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} +1 & +1 \\ -1 & +1 \end{pmatrix}.$$

$$U|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \cdot (\alpha|0\rangle + \beta|1\rangle)$$

$$= \left(\frac{\alpha+\beta}{\sqrt{2}}\right)|0\rangle - \left(\frac{\alpha-\beta}{\sqrt{2}}\right)|1\rangle$$

Meas. in $|0\rangle, |1\rangle$ (Z) basis:

0 w/ prob. $\frac{|\alpha+\beta|^2}{2}$

1 w/ prob. $\frac{|\alpha-\beta|^2}{2}$

$\Rightarrow$ Y transforms (almost...) between X and Z basis!

(i.e.: X meas. can be realized as evolution + Z meas.)

<u>Note:</u> Seq. meas. of $Z \to X \to Z$ will give a <u>random outcome</u> for 2nd Z meas.

$\Rightarrow$ X and Z cannot be measured simultaneously ($\Rightarrow$ uncertainty!)

<u>Measurement on a bipartite state:</u>

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right)$$

Alice measures Z, Bob measures Z:

Projectors $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

$\Rightarrow$ 01 and 10 w. prob $1/2$

Alice measures X, Bob meas. X:

Projectors $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$:

(use $\langle +|0\rangle = \langle +|1\rangle = \langle -|0\rangle = 1/\sqrt{2}$; $\langle -|1\rangle = -1/\sqrt{2}$)

$$|\langle ++|\psi\rangle|^2 = 0$$

$$|\langle +-|\psi\rangle|^2 = \left|-\frac{1}{2\sqrt{2}} - \frac{1}{2\sqrt{2}}\right|^2 = \frac{1}{2}$$

$$|\langle -+|\psi\rangle|^2 = \ldots = \frac{1}{2}$$

$$|\langle --|\psi\rangle|^2 = \ldots = 0$$

$\Rightarrow$ anticorrelation

In fact, anti-corr in <u>all</u> basis (HW)

Alice meas. X, Bob meas. Z:

$$\left.\begin{aligned} |\langle +0|\psi\rangle|^2 &= \left|-\tfrac{1}{2}\right|^2 = \tfrac{1}{4} \\ |\langle +1|\psi\rangle|^2 &= \left|\tfrac{1}{2}\right|^2 = \tfrac{1}{4} \\ |\langle -0|\psi\rangle|^2 &= \tfrac{1}{4} \\ |\langle -1|\psi\rangle|^2 &= \tfrac{1}{4} \end{aligned}\right\} \quad \underline{\text{no correlation!}}$$

All meas. for Alice and Bob look random, <u>but</u> their outcomes in the <u>same basis</u> are perfectly anti-correlated!

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2. <u>Mixed states</u>

Consider bipartite state $|\psi\rangle_{AB}$. We only have access to A.

e.g. $|\psi\rangle_{AB} = c_{00}|0\rangle|0\rangle + c_{01}|0\rangle|1\rangle + c_{10}|1\rangle|0\rangle + c_{11}|1\rangle|1\rangle$.

Can we characterize measurement outcomes on A in a simple way?

A measures $M \rightarrow$ joint measurement $M_A \otimes I_B$

$$\langle\psi|M_A \otimes I_B|\psi\rangle = \sum c^*_{i'j'} \langle i'|\langle j'| (M_A \otimes I_B)\, c_{ij} |i\rangle|j\rangle$$

$$= \sum c^*_{i'j'} c_{ij} \langle i'|M_A|i\rangle \underbrace{\langle j'|j\rangle}_{=\delta_{jj'}}$$

$$= \sum' \langle i'|\Pi|i\rangle \, c^*_{i'j} \, c_{ij}$$

$$= \mathrm{tr}\left[\Pi \left(\sum |i\rangle\langle i'| \, c_{ij} \, c^*_{i'j} \right) \right] = \underline{\mathrm{tr}\left[\Pi \rho_A \right]}$$

(*) with $\rho_A = \sum' c_{ij} c^*_{i'j} \, |i\rangle\langle i'|$ the <u>density operator</u> or <u>density matrix</u>

and the <u>trace</u> $\mathrm{tr}[X] = \sum' \langle k|X|k\rangle$.

Note that the trace is <u>cyclic</u>:

$$\underline{\mathrm{tr}[AB]} = \sum_k \langle k|AB|k\rangle = \sum_{kl} \langle k|A|l\rangle\langle l|B|k\rangle$$

un-square

$$= \sum \langle l|B|k\rangle \langle k|A|l\rangle = \underline{\mathrm{tr}[BA]}.$$

<u>Density operator</u>: Characterization of system w/ only partial knowledge.

What are the properties of ρ_A? Use (*):

$$\rho_A^\dagger = \sum \left(c_{ij} c^*_{i'j}\right)^* |i'\rangle\langle i| = \sum c_{i'j} c^*_{ij} |i'\rangle\langle i| = \rho_A$$

$$\langle\phi|\rho_A|\phi\rangle = \sum c_{ij} c^*_{i'j} \underbrace{\langle\phi|i\rangle}_{a_i^*} \underbrace{\langle i'|\phi\rangle}_{a_{i'}}$$

$$= \sum_j \left(\sum_i a_i^* c_{ij}\right)\left(\sum_{i'} a_{i'} c^*_{i'j}\right) = \sum w_j^* w_j \geq 0.$$

$\Rightarrow \rho_A \geq 0$ (i.e., ρ_A has only non-negative eigenvalues: it is <u>positive semidefinite</u>)

$$\mathrm{tr}[\rho_A] = \sum_k \sum_{i i' j} c_{ij} c_{i'j}^* \underbrace{\langle k | i \rangle \langle i' | k \rangle}_{= \delta_{ik} \delta_{i'k}} = \sum c_{kj} c_{kj}^* = 1 .$$

<u>Properties of density operators:</u>

- $\rho_A^\dagger = \rho_A$
- $\rho_A \geq 0$
- $\mathrm{tr}(\rho_A) = 1$.

(Note: the ρ_A form a convex set S, i.e.: $\rho, \sigma \in S \Rightarrow p\rho + (1-p)\sigma \in S$, $0 \leq p \leq 1$)

<u>We will see:</u> This provides an <u>alternative fundamental</u> definition of a state (i.e., <u>all</u> ρ_A of the above form arise if we only have access to part of a system.)

If state of A is <u>pure</u>, i.e., $|\psi\rangle = |\phi_A\rangle \otimes |\chi_B\rangle$

$$\Rightarrow \rho_A = |\phi_A\rangle\langle\phi_A|$$

(can be seen e.g. by writing everything in a basis which contains $|\phi_A\rangle$ and $|\chi_B\rangle$, resp., and use basis independence.)

Note: For a given state $|\psi\rangle_{AB}$, the ρ_A for which

$$\mathrm{tr}[\Pi \rho_A] = \langle\psi|\Pi\otimes I|\psi\rangle$$

is uniquely determined (since its Hilbert-Schmidt scalar product w. all Hermitian Π is determined).

$\Longrightarrow$ all numbers in ρ_A are meaningful (unlike the phase of a pure state vector) — "nicer" than for pure states

Partial trace:

Imagine A+B are mixed: ρ_{AB}.

Description of measurement Π on A?

$$\mathrm{tr}\left[(\Pi\otimes I)\rho_{AB}\right] = \sum \underbrace{\langle ij|\Pi\otimes I|i'j'\rangle}_{\delta_{jj'}}\langle i'j'|\rho_{AB}|ij\rangle$$

$$= \sum \langle i|\Pi|i'\rangle\langle i'j|\rho_{AB}|ij\rangle$$

$$= \mathrm{tr}\left[\Pi\cdot\rho_A\right]$$

with $\rho_A = \sum |i'\rangle\langle i'j|\rho_{AB}|ij\rangle\langle i|$

$= \ldots$

$$= \sum \mathbb{1}_A \otimes \langle j|_B (\rho_{AB}) \ \mathbb{1}_A \otimes |j\rangle_B$$

$$= \sum \langle j|_B \, \rho_{AB} \, |j\rangle_B$$

$$= \mathrm{tr}_B \, \rho_{AB} \quad : \quad \text{"}\underline{\text{partial trace}}\text{"}$$

In components:

$$\left(\mathrm{tr}_B \, \rho_{AB}\right)_{ii'} = \sum_j \left(\rho_{AB}\right)_{(ij)(i'j)}$$

<u>Interpretation of density matrix:</u>

Consider $|\psi\rangle = \alpha|00\rangle + \beta|11\rangle$

$$\Rightarrow \quad \rho_A = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix} = |\alpha|^2 |0\rangle\langle 0| + |\beta|^2 |1\rangle\langle 1|$$

$$\mathrm{tr}\left[\Pi \rho_A\right] = |\alpha|^2 \langle 0|\Pi|0\rangle + |\beta|^2 \langle 1|\Pi|1\rangle$$

$\Rightarrow$ can be interpreted as having $|0\rangle$ w/ $p_0 = |\alpha|^2$ and $|1\rangle$ w/ $p_1 = |\beta|^2$: "ensemble interpretation"

<u>But</u>: State of A+B pure : consistent interpretation?

B can prepare ensemble by proj. meas. in Z basis:

$$
|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \;\xrightarrow[\text{on } B]{Z\text{ meas.}}\;
\begin{cases}
p_0 = |\alpha|^2: & |\psi_0\rangle_A = |0\rangle_A \\
p_1 = |\beta|^2: & |\psi_1\rangle_A = |1\rangle_A
\end{cases}
$$

$\Longrightarrow$ ensemble $\rho_A = \{(p_0, |0\rangle), (p_1, |1\rangle)\}$ for Alice.

Bob knows which state Alice holds!

$\rightarrow$ Bob's description of Alice's state is
either $|0\rangle$ or $|1\rangle$, not ρ_A!

$\rightarrow$ Description of q. state depends on knowledge!

But: Bob could do a different measurement, e.g. in the $|\pm\rangle$ basis!

$$
|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \;\xrightarrow[\text{on } B]{X\text{ meas.}}\;
\left.\begin{cases}
p_+ = \dfrac{|\alpha|^2+|\beta|^2}{2} = \dfrac{1}{2}: & |\psi_+\rangle_A = \dfrac{\alpha|0\rangle + \beta|1\rangle}{|\alpha|^2+|\beta|^2} \\[2ex]
p_- = \dfrac{|\alpha|^2+|\beta^2|}{2} = \dfrac{1}{2}: & |\psi_-\rangle_A = \dfrac{\alpha|0\rangle - \beta|1\rangle}{|a|^2+|\beta|^2}
\end{cases}\right\} \text{non-orthogonal!}
$$

$$\rho_A = p_+ |\psi_+\rangle\langle\psi_+| + p_- |\psi_-\rangle\langle\psi_-|$$

$\Longrightarrow$ Different ensemble interpretation of same state.

$\Rightarrow$ <u>ambiguity</u> of ensemble interpretation!

In fact, there are <u>infinitely many</u> ensembles for the same density operator!

Even the number of terms can vary:

E.g.: $$|\psi\rangle = \frac{\alpha|00\rangle + \beta|11\rangle}{\sqrt{2}} + \frac{\alpha|02\rangle + \beta|13\rangle}{\sqrt{3}}$$

Measure in basis $|0\rangle, |1\rangle, \frac{|2\rangle \pm |3\rangle}{\sqrt{2}} =: |\pm\rangle$

$\rightarrow$ combination of the two previous schemes!

$$\Rightarrow \quad \rho_A = \underset{\substack{\parallel \\ |\alpha|^2/2}}{p_0} |0\rangle\langle 0| + \underset{\substack{\parallel \\ |\beta|^2/2}}{p_1} |1\rangle\langle 1| + \underset{\substack{\parallel \\ 1/4}}{p_+} |\psi_+\rangle\langle\psi_+| + \underset{\substack{\parallel \\ 1/4}}{p_-} |\psi_-\rangle\langle\psi_-|$$

How are different ensembles related?

<u>Theorem</u>: Let $\rho = \sum p_i |\psi_i\rangle\langle\psi_i| = \sum q_j |\phi_j\rangle\langle\phi_j|$.

Then, there is a unitary $U = (u_{ij})$ s.th.

$$\sqrt{p_i}|\psi_i\rangle = \sum u_{ij} \sqrt{q_j}\, |\phi_j\rangle,$$

and vice versa. (If the number of i's and j's is different, pad the smaller one with zero vectors!)

Proof:

"$\Leftarrow$": Let $\sqrt{p_i}\,|\psi_i\rangle = \sum u_{ij}\sqrt{q_j}\,|\phi_j\rangle$.

Then $$\sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i \Big(\sum_j u_{ij}\sqrt{q_j}\,|\phi_j\rangle\Big)\Big(\sum_{j'} u_{ij'}^*\sqrt{q_{j'}}\langle\phi_{j'}|\Big)$$

$$= \sum_{jj'} \sqrt{q_j}\,|\phi_j\rangle\langle\phi_{j'}|\sqrt{q_{j'}}\;\underbrace{\Big(\sum_i u_{ij'}^* u_{ij}\Big)}_{=\delta_{jj'}}$$

$$= \sum_j q_j\,|\phi_j\rangle\langle\phi_j|$$

"$\Rightarrow$": First, assume $|\phi_j\rangle$ is an eigenbasis. Define

$$u_{ij} = \langle\phi_j|\psi_i\rangle \cdot \frac{\sqrt{p_i}}{\sqrt{q_j}}$$

Then, $$\sum_j u_{ij}\sqrt{q_j}\,|\phi_j\rangle = \sum_j \sqrt{q_j}\,|\phi_j\rangle\langle\phi_j|\psi_i\rangle\,\frac{\sqrt{p_i}}{\sqrt{q_j}} = \sqrt{p_i}\,|\psi_i\rangle$$

and $$\sum_i u_{ij} u_{ij'}^* = \sum_i \langle\phi_j|\psi_i\rangle\langle\psi_i|\phi_{j'}\rangle\,\frac{p_i}{\sqrt{q_j q_{j'}}}$$

$$= \underbrace{\langle\phi_j|\rho|\phi_{j'}\rangle}_{=q_j\delta_{jj'}}\,\frac{1}{\sqrt{q_j q_{j'}}} = \delta_{jj'}$$

$\Rightarrow$ u_{ij} has orthogonal columns $\Rightarrow$ can be extended to unitary (by padding $|\phi_i\rangle$ with zero vectors).

General case: Go via eigenbasis & combine unitaries! $\square$

3. Schmidt decomposition and purifications

Consider bipartite state $|\psi\rangle_{AB}$, and let

$$\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A = \sum p_i |i\rangle_A\langle i|_A \Rightarrow |i\rangle_A \text{ ONB}.$$

Choose an ONB $|a_j\rangle_B$ for B, and expand

$$|\psi\rangle_{AB} = \sum c_{ij} |i\rangle_A |a_j\rangle_B$$

$$= \sum |i\rangle_A |b_i\rangle_B \quad , \quad \underbrace{|b_i\rangle}_{\text{no ONB!}} = \sum c_{ij} |a_j\rangle$$

Now $\sum p_i |i\rangle\langle i| = \mathrm{tr}_B |\psi\rangle\langle\psi| = \mathrm{tr}_B \left(\sum_{ii'} |i\rangle\langle i'|_A \, |b_i\rangle\langle b_{i'}|_B \right)$

$$= \sum_{j,ii'} |i\rangle\langle i'| \underbrace{\langle a_j|b_i\rangle\langle b_{i'}|a_j\rangle}_{\sum_j : \; = \langle b_{i'}|b_i\rangle}$$

$$= \sum \langle b_{i'}|b_i\rangle \; |i\rangle\langle i'|$$

$|i\rangle\langle i'|$ is a basis for the space of matrices (= linear maps):

$$\Rightarrow \langle b_{i'}|b_i\rangle = \delta_{i'i} \, p_i$$

$\Rightarrow$ $|i\rangle_B := \frac{1}{\sqrt{p_i}} |b_i\rangle$ is ONB for B

different from $|i\rangle_A$!

$$\Rightarrow \boxed{\begin{gathered} |\psi\rangle_{AB} = \sum_i \sqrt{p_i}\, |i\rangle_A |i\rangle_B \\ \text{with } |i\rangle_A,\ |i\rangle_B \text{ ONBs} \end{gathered}}$$

"Schmidt decomposition" with Schmidt coefficients $\sqrt{p_i}$.

Note: $\rho_B = \mathrm{tr}_A |\psi\rangle\langle\psi| = \sum_i p_i |i\rangle_B\langle i|_B$

$\Rightarrow$ $|i\rangle_B$ is the eigenbasis of ρ_B !

p_i non-degenerate $\Rightarrow$ Schmidt decomposition obtained by pairing up eigenvectors of ρ_A and ρ_B !

Important consequence: Eigenvalues of ρ_A and ρ_B are equal !

How is the Schmidt decomp. related to other expansions?

$$|\psi\rangle = \sum c_{ij} \underbrace{|x_i\rangle_A |y_j\rangle_B}_{\text{ONB}}$$

$$= \sum \sqrt{p_k}\, |k\rangle_A |k\rangle_B$$

$\Longrightarrow$ $\exists$ unitaries u_{ik}, v_{jk} s.th.

$$|k\rangle_A = \sum u_{ik} |x_i\rangle_A ; \quad |k\rangle_B = \sum v_{jk}^* |y_j\rangle_B$$

(pad p_k w/ zeros if necessary).

$\xRightarrow[\text{+ lin. indep.}]{\text{input above}}$

$$c_{ij} = \sum_k u_{ik} \sqrt{p_k}\, v_{jk}^* ,$$

or

$$C = \underset{(u_{ik})}{U} \cdot \underset{\begin{pmatrix}\sqrt{p_1} & \\ & \ddots\end{pmatrix}}{D} \cdot \underset{(v_{jk})}{V^\dagger} ; \quad U, V \text{ unitary}, \; D \text{ diagonal}$$

$$\boxed{\text{"singular value decomposition" (SVD)}}$$

<u>Remark</u>: Any two states $|\phi\rangle, |\psi\rangle$ w/ identical Schmidt coefficients are related by local unitaries, i.e.:

$$\exists U, V \text{ s.th. } |\phi\rangle = (U \otimes V)|\psi\rangle.$$

<u>I.e.</u>: All non-local properties are encoded in the p_i!

<u>Proof</u>:
$$|\phi\rangle = \sum \sqrt{p_i}\, |\phi_i^A\rangle \otimes |\phi_i^B\rangle$$
$$|\psi\rangle = \sum \sqrt{p_i}\, |\psi_i^A\rangle \otimes |\psi_i^B\rangle$$

$|\phi_i^A\rangle, |\psi_i^A\rangle$ orthonormal $\Rightarrow \exists U : |\phi_i^A\rangle = U|\psi_i^A\rangle\ \forall i$

$|\phi_i^B\rangle, |\psi_i^B\rangle$ —"— $\Rightarrow \exists V : |\phi_i^B\rangle = V|\psi_i^B\rangle\ \forall i$

$\boxed{R}$

(Note: If necessary, we have to pad the p_i with zeros and embed Hilbert space in larger one.)

<u>Purifications</u>:

Have seen: Bipartite state $|\psi\rangle_{AB}$ w/ access to A only

$\Rightarrow$ described by ρ_A, $\rho_A \geq 0$, $\mathrm{tr}\,\rho_A = 1$

Will now show: <u>Any</u> such ρ_A can be seen as arising from $|\psi\rangle_{AB}$ ("purification")

Let $\rho = \sum p_i |\phi_i\rangle\langle\phi_i|$ ← need not be orthogonal

Choose $|\psi\rangle_{AB} = \sum \sqrt{p_i}\, |\phi_i\rangle_A |i\rangle_B$ ← orthonormal.

Then $tr_B |\psi\rangle\langle\psi| = \sum_{k,i,j} \underbrace{\langle k|_B \Big(\sqrt{p_i p_j}\, |\phi_i\rangle_A |i\rangle_B}_{=\delta_{ki}} \langle\phi_j|_A \underbrace{\langle j|_B \Big) |k\rangle_B}_{=\delta_{kj}}$

$= \sum_k p_k |\phi_k\rangle\langle\phi_k|$ ✓

$|\psi\rangle$ is called <u>purification</u> of ρ.

<u>Notes:</u>
- Measuring in basis $|i\rangle_B$ prepares ensemble $\{p_i, |\phi_i\rangle\}$
- We can always choose $\dim(\mathcal{H}_B) \le \dim(\mathcal{H}_A)$ by using eigenvalue decomposition of ρ.
  (In fact, even $\dim \mathcal{H}_B$ = # non-zero Schmidt coeffs.)

Many different purifications exist! How are they related?

Let $|\phi\rangle_{AB}$, $|\psi\rangle_{AB}$ be purifications of ρ_A.

Write both in their Schmidt decomposition:

$$|\phi\rangle = \sum_{i} \lambda_i \, |\phi_i^A\rangle |\phi_i^B\rangle$$

$$|\psi\rangle = \sum \lambda_i \, |\psi_i^A\rangle |\psi_j^B\rangle.$$

We have $\sum \lambda_i |\phi_i^A\rangle\langle\phi_i^A| = \sum \lambda_i |\psi_i^A\rangle\langle\psi_i^A|$

$\Longrightarrow$ $|\phi_i^A\rangle = |\psi_i^B\rangle$ if λ_i non-degenerate

<u>and we know</u> from construction of Schmidt decomp.

that we can choose $|\phi_i^A\rangle = |\psi_i^A\rangle$ $\forall i$!

Now choose U s.th. $U|\phi_i^B\rangle = |\psi_i^B\rangle$ $\forall i$.

$$\Longrightarrow \quad |\psi\rangle = (\mathbb{1} \otimes U)\, |\phi\rangle.$$

All purifications are related by a unitary on the purifying system.

(<u>Note</u>: This can be seen as a reformulation of the unitary relation of ensemble decompositions.)

4.1. Unitary evolution of mixed states

How does a mixed state ρ_A evolve under a unitary U_A?

Consider purification $|\psi\rangle_{AB}$; $\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A$.

$$|\psi\rangle \longmapsto (U_A \otimes \mathbb{1}_B)|\psi_{AB}\rangle$$

$$\Rightarrow \rho_A = \mathrm{tr}_B |\psi\rangle\langle\psi| \longmapsto \mathrm{tr}_B \left[(U_A \otimes \mathbb{1}_B)|\psi_{AB}\rangle\langle\psi_{AB}|(U_A^\dagger \otimes \mathbb{1}_B)\right]$$

$$= U_A \cdot \mathrm{tr}_B \left[(\mathbb{1}_A \otimes \mathbb{1}_B)|\psi_{AB}\rangle\langle\psi_{AB}|(\mathbb{1}_A \otimes \mathbb{1}_B)\right] U_A^\dagger$$

$$= \underline{\underline{U_A \rho_A U_A^\dagger}}.$$

2. Measurement of mixed states

Projective measurement E_n:

Have seen: $p_n = \mathrm{tr}[E_n \rho_A]$.

Post-measurement state:

$$\rho_{A,n} = \frac{1}{p_n} \mathrm{tr}_B \left((E_n \otimes \mathbb{1})|\psi\rangle\langle\psi|(E_n^\dagger \otimes \mathbb{1})\right)$$

$$= \underline{\underline{\frac{1}{p_n} E_n \rho_A E_n^\dagger}}$$

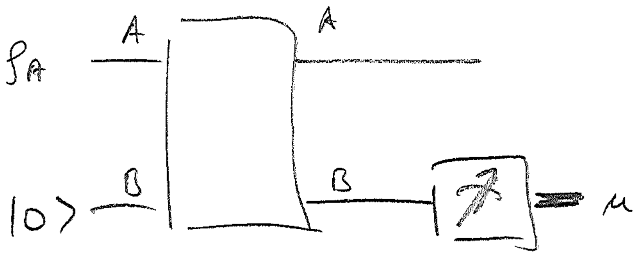
4. POVM measurements

Have seen: additional system B → more rich situation

What measurements can we do by adding an extra system?

Idea:

Add "ancilla" B (in state $|0\rangle_B$), act w/ unitary on AB, and measure B in computational basis $|0\rangle, \dots, |d-1\rangle$.



Post-measurement state (unnormalized):

$$\tilde{\rho}_u^A = \langle u|_B\, U \left(\rho_A \otimes |0\rangle_B\langle 0|_B\right) U^\dagger |u\rangle_B$$

$$= M_u\, \rho_A\, M_u^\dagger, \quad \text{with } M_u := \langle u|_B\, U\, |0\rangle_B .$$

$$\equiv \left(\mathbb{1}_A \otimes \langle u|_B\right) U \left(\mathbb{1}_A \otimes |u\rangle_B\right)$$

and $p_u = tr\left(\tilde{\rho}_u^A\right) = tr\left(M_u \rho_A M_u^\dagger\right) = tr\left(M_u^\dagger M_u \rho_A\right)$

$\rho_u^A = \frac{1}{p_u}\tilde{\rho}_u^A$ post-meas. state.

What properties does Π_u have?

$$\underline{\underline{\sum \Pi_u^\dagger \Pi_u}} = \sum_u \langle 0|_B \, \underbrace{U \, \underbrace{|u\rangle_B \langle u|_B}_{=\mathbb{1}} \, U}_{=\mathbb{1}} |0\rangle_B = \langle 0|_B \mathbb{1}_{AB} |0\rangle_B$$

$$= \underline{\underline{\mathbb{1}_A}}.$$

(Also follows from $1 = \sum p_u = \sum \mathrm{tr}(\Pi_u^\dagger \Pi_u \rho_A) = \mathrm{tr}(\sum \Pi_u^\dagger \Pi_u \rho_A)$ $\forall \rho_A$)

A set of $\{\Pi_u\}$ (or $\{\Pi_u^\dagger \Pi_u\}$ w/ $\sum \Pi_u^\dagger \Pi_u = \mathbb{1}$ is called a "positive operator-valued measure" (POVM), and the corresp. measurement a <u>POVM measurement</u>.

Can any set Π_u w/ $\sum \Pi_u^\dagger \Pi_u = \mathbb{1}$ be realized by extensions + unitaries?

$$\begin{pmatrix} \Pi_0 \\ \vdots \\ \\ \Pi_{d-1} \end{pmatrix} \quad \overset{\sum \Pi_u^\dagger \Pi_u = \mathbb{1}}{\Longrightarrow} \quad \text{matrix w/ orthogonal columns} \quad \Longrightarrow \quad \ldots$$

$\Rightarrow$ can be extended to unitary U

$$U = \begin{array}{c} \\ \langle 0|_B \\ \langle 1|_B \\ \vdots \\ \langle d-1|_B \end{array} \begin{array}{c} |0\rangle_B \\ \left(\begin{array}{c|cccc} M_0 & \cdot & \cdot & \cdot & \cdot \\ \hline M_1 & \cdot & \cdot & \cdot & \cdot \\ \hline \vdots & & & & \\ \hline M_{d-1} & \cdot & \cdot & \cdot & \cdot \end{array} \right) \end{array}$$

i.e.: $\langle n|_B \, U \, |0\rangle_B = M_n$.

$\Rightarrow$ measurement $\{M_n\}$ can be realized by unitary U & projective measurement!

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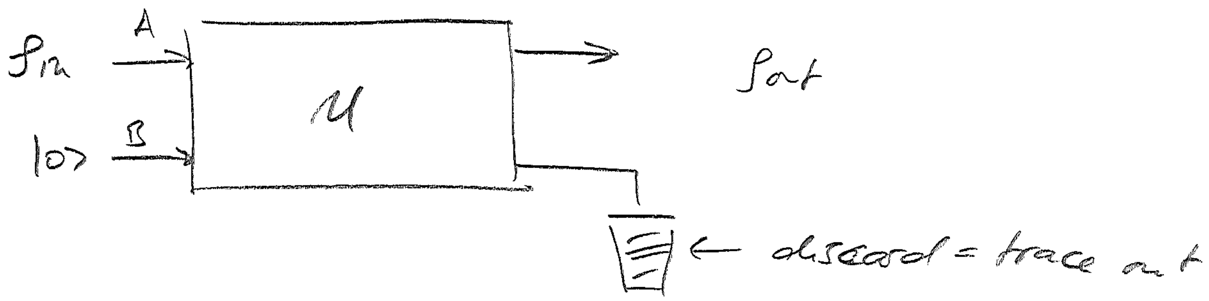
5. General evolution – superoperators

What evolutions can we realize by evolving a larger system with a unitary?



$$\rho \mapsto \mathcal{E}(\rho) = \mathrm{tr}_B\left[U (\rho \otimes |0\rangle\langle 0| U^\dagger \right]$$

$$= \sum {}_B\langle u| U |0\rangle_B \; \rho \; {}_B\langle 0| U^\dagger |u\rangle_B$$

$$= \sum M_u \rho M_u^\dagger \; ; \quad \text{with} \quad M_u = {}_B\langle u| U |0\rangle_B .$$

(Note: Trace in any basis $|\tilde{m}\rangle = \sum v_{mu} |u\rangle$, v unitary:

M_u and $\tilde{M}_m = \sum v^\dagger_{mu} M_u$ describe <u>same evolution</u>.)

Properties of M_u?

As before: $\sum M_u^\dagger M_u = \sum {}_B\langle 0| U^\dagger |u\rangle_B \, {}_B\langle u| U |0\rangle_B = \mathbb{1}_A$.

> We call a <u>physical map</u> between density matrices a <u>superoperator</u>, and the form
>
> $$\mathcal{E} : \rho \mapsto \sum M_u \rho M_u^\dagger ; \quad \sum M_u^\dagger M_u = \mathbb{1}$$
>
> its <u>Kraus representation</u>.

<u>Note</u>: Any map of the form $\rho \mapsto \sum M_u \rho M_u^\dagger$ can be implemented via unitary + tracing out (cf. POVMs). In fact, $\mathcal{E}$ can be considered as a POVM meas. w/out knowing the result ("measurement by environment")

What is the most general physical evolution $\mathcal{E}$?

Properties:

- hermiticity-preserving: $\rho = \rho^\dagger \Rightarrow \mathcal{E}(\rho) = \mathcal{E}(\rho^\dagger)$
- positive: $\rho \geq 0 \Rightarrow \mathcal{E}(\rho) \geq 0.$
- trace-preserving: $\mathrm{tr}(\rho) = 1 \Rightarrow \mathrm{tr}(\mathcal{E}(\rho)) = 1$
- linearity: $\mathcal{E}(\rho + \lambda\sigma) = \mathcal{E}(\rho) + \lambda\,\mathcal{E}(\sigma).$

Do we need linearity?

$\rightarrow$ Yes, otherwise ensemble interpretation becomes inconsistent! ($\rightarrow$ Homework)

Is this enough for a physical map?

<u>No</u>. Want that $\mathcal{E}$ acts as a physical map even on part of a larger system:

$\boxed{\text{"complete positivity"}}$

$$\rho_{AB} \geq 0 \Rightarrow (\underbrace{\mathcal{E}_A \otimes \mathbb{1}_B}) (\rho_{AB}) \geq 0$$

$\boxed{\begin{array}{l}\text{\underline{Note}: } \mathcal{E}_A \otimes \mathbb{1}_B \text{ is defined using linearity on a basis:} \\ \qquad (\mathcal{E}_A \otimes \mathbb{1}_B)(M \otimes N) = \mathcal{E}_A(M) \otimes N.\end{array}}$

We call $\mathcal{E}$ a completely positive trace preserving (CPTP) map (or "quantum channel").

Are there maps which are positive but not CP?

Yes: E.g. "transpose channel":

$$\mathcal{E} : \rho \longmapsto \rho^T$$

$$(\mathcal{E} \otimes \mathbb{1})(\rho_{AB}) = \rho^{T_A} \quad \text{; "partial transposition"}$$

E.g.: $|\Omega\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|0\rangle + |1\rangle|1\rangle\right)$

$$(|\Omega\rangle\langle\Omega|)^{T_B} = \frac{1}{2}\left(|00\rangle\langle 00| + |01\rangle\langle 10| + |10\rangle\langle 01| + |11\rangle\langle 11|\right)$$

$$\hat{=} \frac{1}{2}\begin{pmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{pmatrix} \not\geq 0.$$

Note: Positive but not completely positive maps are very important as "entanglement witnesses": $(\mathcal{E}\otimes\mathbb{1})(\rho) \geq 0$ for all unentangled states, but $(\mathcal{E}\otimes\mathbb{1})(\sigma) \not\geq 0$ can "witness" certain entangled states σ.

Are all CPTP maps of Kraus form?

The Choi-Jamiołkowski isomorphism:

Let $\mathcal{E}$ be CPTP.

Define $\sigma_{AB} = (\mathcal{E} \otimes \mathbb{1})(|\Omega\rangle\langle\Omega|)$; $|\Omega\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle|i\rangle$.

Then, $\sigma_{AB} \geq 0$, and

$$\mathrm{tr}_A(\sigma_{AB}) = \frac{1}{d} \sum_{ij} \mathrm{tr}_A\big(\underbrace{\mathcal{E}_A(|i\rangle\langle j|)}_{=\delta_{ij}} \otimes |i\rangle\langle j|_B\big) = \frac{1}{d}\mathbb{1}$$

the "Choi-Jamiołkowski state" of $\mathcal{E}$.

We have

$$d\,\mathrm{tr}_B[\sigma_{AB}\rho_B^T] = \sum_{ij} \mathrm{tr}_B[\mathcal{E}(|i\rangle\langle j|) \otimes |i\rangle\langle j| \rho_B^T]$$

$$= \sum_{ij} \mathcal{E}(|i\rangle\langle j|) \cdot \underbrace{\langle j|\rho_B^T|i\rangle}_{=\rho_{ij}} = \mathcal{E}(\rho_B)$$

and

$$\mathrm{tr}_A(d\,\mathrm{tr}_B[\sigma_{AB}\rho_B^T]) = d\,\mathrm{tr}_B[\mathrm{tr}_A(\sigma_{AB}\rho_B^T)]$$

$$= d\,\mathrm{tr}_B\big(\underbrace{(\mathrm{tr}_A \sigma_{AB})}_{\stackrel{!}{=} \frac{1}{d}\mathbb{1}} \rho_B^T\big)$$

$\Rightarrow$ trace-preserving iff $\mathrm{tr}_A \sigma_{AB} = \frac{1}{d}\mathbb{1}$.

Isomorphism ("Choi-Jamiołkowski isomorphism") between superoperators $\mathcal{E}: \mathcal{B}(\mathbb{C}^d) \longrightarrow \mathcal{B}(\mathbb{C}^d)$

and states $\sigma_{AB} \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$; $\sigma_{AB} \geq 0$.

Moreover: $\mathcal{E}$ T.P. iff $tr_A\, \sigma_{AB} = \frac{1}{d} \mathbb{1}$.

Back to: Is any superoperator of Kraus form?

Let σ_{AB} be its C-J state.

$$\Rightarrow \quad \sigma = \sum |\tilde{\psi}_k\rangle\langle\tilde{\psi}_k| \quad \leftarrow \text{unnormalized.}$$

Write $|\tilde{\psi}_k\rangle = \sum_{ij} m_k^{ij} |j\rangle|i\rangle = \frac{1}{\sqrt{d}} \sum_i (M_k \otimes \mathbb{1})|i\rangle|i\rangle = (M_k \otimes \mathbb{1})|\Omega\rangle$ ← ONB

$$\Rightarrow \quad \sigma = \sum M_k |\Omega\rangle\langle\Omega| M_k^\dagger ; \quad \text{and}$$

$$\mathcal{E}(\rho) = d\, tr_B \Big[\sum_k (M_k \otimes \mathbb{1}) |\Omega\rangle\langle\Omega| (M_k^\dagger \otimes \mathbb{1}) (\mathbb{1} \otimes \rho^T) \Big] = d \sum_k M_k \underbrace{tr_B \big[|\Omega\rangle\langle\Omega| \rho^T \big]}_{(*)} M_k^\dagger ,$$

$$\boxed{(*) = \frac{1}{d} \sum_{ij} |i\rangle\langle j| \underbrace{tr_B \big[|i\rangle\langle j| \rho^T \big]}_{= \rho_{ij}} = \frac{1}{d} \rho}$$

$$= \sum_k M_k \rho M_k^\dagger .$$

Furthermore:

$$\mathbb{1} = \mathrm{tr}_A\, \sigma = \mathrm{tr}_A \sum_k (\Pi_k \otimes \mathbb{1}) |\Omega\rangle\langle\Omega| (\Pi_k^\dagger \otimes \mathbb{1})$$

$$= \sum_k \mathrm{tr}_A (\Pi_k^\dagger \Pi_k \cdot |\Omega\rangle\langle\Omega|)$$

$$= \sum_k \mathrm{tr}\,(\Pi_k^\dagger \Pi_k |i\rangle\langle j|) \otimes |i\rangle\langle j|$$

$$\Longrightarrow \quad \langle j| \sum_k \Pi_k^\dagger \Pi_k |i\rangle = \delta_{ij}$$

$$\longrightarrow \quad \sum_k \Pi_k^\dagger \Pi_k = \mathbb{1}$$

$\Longrightarrow$ All superoperators are of Kraus form.

$\sum_k \Pi_k^\dagger \Pi_k$ corresponds to trace-preserving.

Note: Non-t.p. maps can be implemented by postselecting on certain measurement outcomes.

6. Axioms ("mixed" version)

- States are linear operators $\rho \in \mathbb{B}(\mathcal{H})$ with

$$\rho = \rho^{+}$$

$$\rho \geq 0$$

$$\mathrm{tr}\,\rho = 0$$

- Evolution is described by trace-preserving completely positive maps

$$\mathcal{E} : \rho \longmapsto \mathcal{E}(\rho) = \sum \Pi_n \rho \Pi_n^{+}$$

with $\sum \Pi_n^{+} \Pi_n = \mathbb{1}$.

- Measurements act as

$$\rho \longrightarrow \rho_n = \frac{\Pi_n \rho \Pi_n^{+}}{\mathrm{tr}(\Pi_n \rho \Pi_n^{+})}$$

with probability $p_n = \mathrm{tr}(\Pi_n^{+} \Pi_n \rho)$,

and $\sum \Pi_n^{+} \Pi_n = \mathbb{1}$.