Freie Universität Berlin
Tutorials on Quantum Information Theory
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Problem Sheet 1
Density matrices and Bell experiments

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1. **Density matrix formulation of Quantum mechanics** (9 points: 1+1+1+2+1+1+2)
The basic ingredients of quantum mechanics are: states, observables and dynamics. In the *density matrix formulation* we can start from the following (incomplete) postulates:

I.) Each physical system is associated with a Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$. The **(mixed) state** of a quantum system is described by a non-negative, self-adjoint linear operator with unit trace, i.e. an element of $\mathcal{D} := \{\rho \in L(\mathcal{H}) \mid \rho = \rho^\dagger,\ \rho \geq 0,\ \operatorname{Tr}\rho = 1\}$.
Remark: *In quantum information theory, it will be sufficient to consider finite dimensional Hilbert spaces most of the time. A finite dimensional Hilbert space is simply a vector space. In infinite dimension there are more subtleties, but these do not concern us.*

II.) **Observables** are represented by Hermitian operators on $\mathcal{H}$. The expectation value of an observable A in the state ρ is given by $\langle A\rangle_\rho = \operatorname{Tr}(A\rho)$.

III.) The **time-evolution** of the state of a quantum system satisfies

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\mathrm{i}[H, \rho],$$

where H is the observable associated to the total energy of the system.

Let us get some geometrical intuition about the set of quantum states.

a) Show that the set $\mathcal{P} = \{\pi \in L(\mathcal{H}) \mid \pi = \pi^\dagger,\ \pi^2 = \pi,\ \operatorname{rank}\pi = 1\}$ of orthogonal projectors onto one-dimensional subspaces of $\mathcal{H}$ is a subset of $\mathcal{D}$.

Most probably, you have originally learned another definition for quantum states in your first quantum mechanics course. Namely, **pure quantum states** are rays of the Hilbert space $\mathcal{H}$. The rays of a Hilbert space are the equivalence classes of unit vector that only differ by a phase factor. In symbols, we have $\operatorname{rays}(\mathcal{H}) = \{|\psi\rangle \in \mathcal{H} \mid \||\psi\rangle\|_2^2 = 1\}/\sim$ with the equivalence relation: $|\psi\rangle \sim |\phi\rangle$ if there exist $\alpha \in \mathbb{R}$ such that $|\psi\rangle = \mathrm{e}^{\mathrm{i}\alpha}|\phi\rangle$. Often physicists tend to drop the equivalence relation and talk about unit vectors as quantum states instead of rays.

b) Show that there is a one-to-one mapping between $\mathcal{P}$ and $\operatorname{rays}(\mathcal{H})$, that is, pure states are equivalent to density matrices that are rank one projectors.

c) Starting from the Schroedinger equation for pure states, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = -\mathrm{i}H|\psi\rangle \tag{1}$$

derive the corresponding evolution equation for density matrices

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\mathrm{i}[H, \rho]. \tag{2}$$

Hint: start by proving this for $\rho = \pi$ a pure state, then use linearity.

d) Define the purity function as $\mathrm{pur}(\rho) := \mathrm{Tr}(\rho^2)$. Show that $\mathrm{pur}(\rho) = 1$ if and only if ρ is pure and that $\frac{1}{d} \leq \mathrm{pur}(\rho) \leq 1$, where d is the dimension of the Hilbert space. What state attains the lower bound? Argue that $\mathrm{pur}(\rho) := \mathrm{Tr}(\rho^2)$ is a measure for the 'purity' of a state $\rho \in \mathcal{D}$. *Hint: for the lower bound, recall the Cauchy Schwarz inequality for the Hilbert Schmidt inner product:* $\mathrm{Tr}(AB^\dagger) \leq \mathrm{Tr}(AA^\dagger)\,\mathrm{Tr}(BB^\dagger)$.

Next, we will see that the generalization to density matrices is a necessary one if we want to study subsystems. Consider a bipartite system AB with Hilbert space $\mathcal{H} = \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$ and an observable $O_A \otimes \mathbb{1}_B$. We will see that the restriction to a subsystem is described by the *partial trace*: For a a linear operator $M : \mathcal{H} \to \mathcal{H}$ this is defined as

$$\mathrm{Tr}_B(M) = \sum_{j=1}^{d_B} (\mathbb{1}_A \otimes \langle j|_B) M (\mathbb{1}_A \otimes |j\rangle_B), \tag{3}$$

where $\{|j\rangle_B\}$ is an arbitrary orthonormal basis (ONB) for $\mathbb{C}^{d_B}$ (as with the trace this definition is independent of the choice of ONB).

e) Show that the partial trace of a state (density operator) is a valid state on the subsystem A.

f) Prove that for any state ρ_{AB} we have

$$\mathrm{Tr}(\rho_{AB} O_A \otimes \mathbb{1}_B) = \mathrm{Tr}(\mathrm{Tr}_B(\rho_{AB}) O_A). \tag{4}$$

for all observables O_A. That is, the partial trace is the *reduced state* on the subsystem A.

g) Reduced states of pure states are not necessarily pure. Let $d_A = d_B =: d$. Show that there is no pure state $|\psi\rangle\langle\psi|_A$ acting on A that satisfies

$$\mathrm{Tr}(\rho_{AB} O_A \otimes \mathbb{1}_B) = \mathrm{Tr}(|\psi\rangle\langle\psi|_A O_A) \tag{5}$$

for $\rho_{AB} = |\Omega_{AB}\rangle\langle\Omega_{AB}|$ and all observables O_A. Here,

$$|\Omega\rangle := d^{-\frac{1}{2}} \sum_{j=1}^{d} |j, j\rangle$$

is the *maximally entangled state*.

2. **An example** (5 points: 2+1+2)
We consider a system with Hilbert space $\mathcal{H} = \mathbb{C}^2$ and basis $\{|0\rangle, |1\rangle\}$. We define the states $\rho_1 = \frac{1}{2}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|)$ and $\rho_2 = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ and the observables $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$ and $X = |0\rangle\langle 1| + |1\rangle\langle 0|$.

a) Is ρ_1 or ρ_2 a pure state, respectively? If this is the case, give the expression of the corresponding ray.

b) Calculate the expectation values $\langle Z\rangle_{\rho_1}$,$\langle Z\rangle_{\rho_2}$,$\langle X\rangle_{\rho_1}$ and $\langle X\rangle_{\rho_2}$.

c) Rewrite ρ_1 and ρ_2 in an eigenbasis of X, i.e. $|+\rangle, |-\rangle$ such that $X|+\rangle = |+\rangle$ and $X|-\rangle = -|-\rangle$. How could you distinguish between ρ_1 and ρ_2 if you did not know which state you had but were allowed to do measurements?

3. **Local and realistic theories** (6 points: 2+2+2)
The violation of so-called Bell inequalities by quantum mechanics lies at the (or rather, a) heart of the way in which quantum information is distinct from classical information. The question we want to answer in this problem is the following: can the randomness of quantum mechanics be explained simply by ignorance of the exact initial state?

To this end we consider an EPR-type setting, in which two parties, Alice and Bob are space-like separated and receive particles sent from and *prepared* by a third party, say, Charlie. Alice and Bob are each capable of performing certain measurements on those particles by adjusting their measurement apparatus.

More precisely, Charlie prepares the particles by randomly choosing a configuration λ of his preparation apparatus with probability $p(\lambda)$ from a configuration space Λ. Λ, λ and p are unknown to Alice and Bob. Upon receiving the particles, Alice and Bob (randomly) choose between two configurations $s \in \mathcal{S} = \{1, 2\}$ of their measurement apparatus and measure the particles, and each of them gets an outcome $A, B \in \{-1, 1\}$.

We now make the following two assumptions about this setting:

- *Realism*: The configuration λ and the measurement setting s uniquely determine the outcome of the measurements. Consequently, we can assign deterministic functions
$$A, B : \mathcal{S} \times \mathcal{S} \times \Lambda \to \{\pm 1\},$$
for Alice's and Bob's measurement, respectively.
- *Locality*: If Alice and Bob are space-like separated, Alice's measurement outcome cannot affect Bob's measurement result and vice versa. This implies that in fact the outcome of A, B only depends on the respective measurement configuration of Alice or Bob so that we can write
$$\begin{aligned} &A : \mathcal{S} \times \Lambda \to \{\pm 1\}; \;\; (s, \lambda) \mapsto A_s(\lambda) \\ &B : \mathcal{S} \times \Lambda \to \{\pm 1\}; \;\; (s, \lambda) \mapsto B_s(\lambda) \end{aligned}$$

Notice that in this setting, the measurement outcomes for Alice and Bob are random, but only because they don't know the exact way in which the state was prepared, λ. If the knew it, they could simply compute $A_s(\lambda)$ or $B_s(\lambda)$ and predict the outcome with certainty. The randomness here is then just a result of ignorance about λ. λ is called a *hidden variable.*

Consider the following expectation value:

$$S = \langle A_1 B_1 + A_2 B_1 + A_1 B_2 - A_2 B_2 \rangle_\lambda \tag{6}$$

Here, $\langle X \rangle_\lambda = \sum_{\lambda \in \Lambda} X(\lambda) p(\lambda)$ is the expectation value of the random variable X that depends on λ.

a) Prove that $|S| \leq 2$ for a local realistic hidden variable setting of the type described above.

Now assume that Charlie does not send an arbitrary pair of particles, but a bipartite quantum state ρ_{AB}, where the first tensor copy is sent to Alice and the second to Bob. The measurements Alice and Bob are allowed to perform are two measurements with outcomes ± 1 each, so $A_i \otimes \mathbb{1}$, and $\mathbb{1} \otimes B_i$, $i = 1, 2$, with A_i, B_i observables on $\mathbb{C}^2$ with spectrum $\{\pm 1\}$. Consider a quantum mechanical version of the previous expectation value:

$$S_{\text{qm}} = \langle A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2 \rangle_\rho, \tag{7}$$

b) Consider the following specific case: $\rho = |\psi\rangle\langle\psi|$ where $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, $A_1 = X, A_2 = Z, B_1 = (X + Z)/\sqrt{2}, B_2 = (X - Z)/\sqrt{2}$. Compute S_{qm}. What do you conclude?

c) Also, consider the case $\rho = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|)$ and $A_1 = X, A_2 = Z, B_1 = (X + Z)/\sqrt{2}, B_2 = (X - Z)/\sqrt{2}$. Compute S_{qm} and compare with the result of the previous point.