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** 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 $\mathcal{D} := \{\rho \in L(\mathcal{H}) \mid \rho = \rho^\dagger,\ \rho \geq 0,\ \operatorname{Tr}\rho = 1\}$. The elements of $\mathcal{D}$ are commonly called *density matrices.*
   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 $\rho$ 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.

   a) Show that if $\rho$ is a convex combination of density matrices $\sigma_i \in \mathcal{D}$, i.e. $\rho = \sum_{i=1}^M p_i\sigma_i$, with probabilities $\sum_i p_i = 1$, then $\rho$ is a density matrix.

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

   b) 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 $\mathcal{D}$. The set $\mathcal{P}$ is called set of *pure-states.*

   c) Show that every density matrix can be written as convex combination of pure states.

   d) 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.*

   e) Define the purity function as $\operatorname{pur}(\rho) := \operatorname{Tr}(\rho^2)$. Show that $\operatorname{pur}(\rho) = 1$ if and only if $\rho$ is pure and that $\frac{1}{d} \leq \operatorname{pur}(\rho) \leq 1$, where $d$ is the dimension of the Hilbert space. What state attains the lower bound? Argue that $\operatorname{pur}(\rho) := \operatorname{Tr}(\rho^2)$ 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:* $\operatorname{Tr}(AB^\dagger)^2 \leq \operatorname{Tr}(AA^\dagger)\operatorname{Tr}(BB^\dagger)$.

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).

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

g) Prove that for any state $\rho_{AB}$ 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 of the combined state $AB$ is the *reduced state* on the subsystem $A$. This is useful because when computing the expectation values of *local* observables one can be concerned only with the part of the system on which the observable acts.

h) 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. **Partial Traces and the Schmidt Decomposition**

We consider a system with Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$. Consider the most general pure state $|\psi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + \delta\,|11\rangle$.

a) Calculate the partial trace $\mathrm{Tr}_2\,|\psi\rangle\langle\psi|$ of its associated density matrix in the basis $\{|0\rangle\langle 0|\,, |0\rangle\langle 1|\,, |1\rangle\langle 0|\,, |1\rangle\langle 1|\}$.

b) Let now $\psi = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, i.e. a Bell state. Use your previous result to show that $\mathrm{Tr}_2\,|\psi\rangle\langle\psi|$ is the maximally mixed state.

c) Let now $|\psi\rangle \in \mathcal{H} \cong \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$ be an arbitrary bipartite pure state. All such states have a Schmidt decomposition $|\psi\rangle = \sum_{i=1}^{\min(d_1,d_2)} \sqrt{\lambda_i}|i\rangle_1|i\rangle_2$, with non-negative real Schmidt values $\lambda_i \in \mathbb{R}_0^+$ and the sets $\{|i\rangle_1\}$, $\{|i\rangle_2\}$ orthonormal bases of $\mathbb{C}^{d_1}$ and $\mathbb{C}^{d_2}$ respectively. Calculate $\mathrm{Tr}_2\,|\psi\rangle\langle\psi|$ in terms of the Schmidt coefficients and basis $\{|i\rangle_1\}$.

d) What condition do the Schmidt coefficients have to satisfy in order for $\mathrm{Tr}_2\,|\psi\rangle\langle\psi|$ to be maximally mixed?

e) Show that if $\mathrm{Tr}_2\,|\psi\rangle\langle\psi|$ is a pure state only a single Schmidt coefficient can be nonzero.

3. **Local and realistic theories**

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 $\lambda$ of his preparation apparatus with probability $p(\lambda)$ from a configuration space $\Lambda$. $\Lambda$, $\lambda$ 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 $\lambda$ 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, $\lambda$. 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 $\lambda$. $\lambda$ 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 $\lambda$.

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 $\rho_{AB}$, 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 $\pm 1$ 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 $S_{\text{qm}}$. 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 $S_{\text{qm}}$ and compare with the result of the previous point.