Freie Universität Berlin
Tutorials on Quantum Information Theory
Winter term 2020/21

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 topological separable complex Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$. The **(mixed) state** of a quantum system is described by a non-negative, self-adjoint (trace-class) 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. From now on, we will always assume that Hilbert spaces are finite-dimensional in the tutorials (if not otherwise stated).*

   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 is given by a differential function $\rho : \mathbb{R} \to \mathcal{D}$ such that

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

   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 $\mathcal{D}$.

   Solution: Let $\pi = U\Lambda U^\dagger$ be the spectral decomposition of π with $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$. Then, $\pi^2 = \pi$ implies that $\lambda_i = \lambda_i^2$ and, hence, $\lambda_i \in \{0, 1\}$ for all i. Thus, $\pi \geq 0$ and furthermore $\operatorname{Tr}\pi = \sum_i \lambda_i = \operatorname{rank}\pi = 1$.

   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 $\operatorname{rays}(\mathcal{H})$.

   Solution: Let $[|\psi\rangle] \in \operatorname{rays}(\mathcal{H})$ and $|\psi\rangle$ be a representative of $[|\psi\rangle]$. We can then associated $|\psi\rangle\langle\psi| \in \mathcal{P}$. This is well-defined since given another represntative $\left|\tilde\psi\right\rangle = \mathrm{e}^{\mathrm{i}\alpha}|\psi\rangle$ with $\alpha \in \mathbb{R}$ we have $\left|\tilde\psi\right\rangle\!\left\langle\tilde\psi\right| = |\psi\rangle\langle\psi|$. Let $\pi \in \mathcal{P}$. The mapping is inverted by choosing a normalised vector from $\operatorname{range}(\pi)$. This choice is unique up to complex phase.

   c) Use this mapping to translate the postulates (I.-III.) to the language of pure states (rays).

Solution:

I.) Each physical system .... The **(pure) states** of a quantum system is described by a ray of the Hilbert space $\mathcal{H}$.

II.) **Observables** .... The expectation value ... is given by $\langle A\rangle_{|\psi\rangle} = \mathrm{Tr}(A\,|\psi\rangle\!\langle\psi| = \langle\psi|A|\psi\rangle$

III.) The **time-evolution** ... differential function $|\psi\rangle : \mathbb{R} \to \mathcal{D}$ such that

$$\frac{\mathrm{d}\,|\psi\rangle\!\langle\psi|}{\mathrm{d}t} = -\mathrm{i}[H, |\psi\rangle\!\langle\psi|] \tag{1}$$

$$\iff \frac{\mathrm{d}\,|\psi\rangle}{\mathrm{d}t}\langle\psi| + |\psi\rangle\frac{\mathrm{d}\,\langle\psi|}{\mathrm{d}t} = -\mathrm{i}\left(H\,|\psi\rangle\langle\psi| - |\psi\rangle\!\langle\psi|\,H\right) \tag{2}$$

$$\iff \frac{\mathrm{d}\,|\psi\rangle}{\mathrm{d}t} = -\mathrm{i}e^{-\mathrm{i}\alpha}H\,|\psi\rangle\,, \tag{3}$$

where $\alpha \in \mathbb{R}$ can be arbitrary. Showing the forward direction of the last step rigorously seems to be not straigt-forward.

d) Argue that $\mathrm{pur}(\rho) := \mathrm{Tr}(\rho^2)$ is a measure for the 'purity' of a state $\rho \in \mathcal{D}$.

Solution: Let $\rho \in \mathcal{D}$ and $(\lambda_1, \dots, \lambda_d) = \mathrm{spec}(\rho)$. Then, $\lambda_i \geq 0$ for all i and by normalisation we have $\sum_i \lambda_i = 1$. Clearly the function $\mathrm{pur}(\rho) = \sum_i \lambda_i^2$ takes its maximal value of 1 only for rank-one projectors. Moreover, its minimal value $1/d$ is realized by the maximally mixed state $\mathbb{1}/d$.

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

$$\mathrm{Tr}_B(M) = \sum_{j=1}^{d_B} (\mathbb{1}_A \otimes \langle j|) M (\mathbb{1}_A \otimes |j\rangle), \tag{4}$$

where $\{|j\rangle\}$ is an arbitrary 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 state on the subsystem A.

Solution: We first observe that taking the adjoint is additive and hence:

$$(\mathrm{Tr}_B(\rho))^\dagger = \left(\sum_{j=1}^{d_B} (\mathbb{1}_A \otimes \langle j|) M (\mathbb{1}_A \otimes |j\rangle)\right)^\dagger \tag{5}$$

$$= \sum_{j=1}^{d_B} ((\mathbb{1}_A \otimes \langle j|) \rho (\mathbb{1}_A \otimes |j\rangle))^\dagger \tag{6}$$

$$= \sum_{j=1}^{d_B} (\mathbb{1}_A \otimes \langle j|) \rho^\dagger (\mathbb{1}_A \otimes |j\rangle) \tag{7}$$

$$= \sum_{j=1}^{d_B} (\mathbb{1}_A \otimes \langle j|) \rho (\mathbb{1}_A \otimes |j\rangle) \tag{8}$$

$$= \mathrm{Tr}_B(\rho). \tag{9}$$

Next, we prove that the trace is preserved under the partial trace:

$$\begin{aligned}
\mathrm{Tr}(\mathrm{Tr}_B(\rho)) &= \mathrm{Tr}\left[\sum_{j=1}^{d_B}(\mathbb{1}_A \otimes \langle j|)M(\mathbb{1}_A \otimes |j\rangle)\right] && (10)\\
&= \sum_{i=1}^{d_A}\langle i|\sum_{j=1}^{d_B}(\mathbb{1}_A \otimes \langle j|)M(\mathbb{1}_A \otimes |j\rangle)|i\rangle && (11)\\
&= \sum_{i=1}^{d_A}\sum_{j=1}^{d_B}(\langle i| \otimes \langle j|)M(|i\rangle \otimes |j\rangle) && (12)\\
&= \mathrm{Tr}(\rho) = 1. && (13)
\end{aligned}$$

Here, the last line follows from observing that $|i\rangle \otimes |j\rangle$ is by definition an ONB for $\mathcal{H}$.

For positivity, we use consider the expectation value

$$\langle\psi|\,\mathrm{Tr}_B(\rho)|\psi\rangle = \mathrm{Tr}(\mathrm{Tr}_B(\rho)|\psi\rangle\langle\psi|) = \mathrm{Tr}(\mathrm{Tr}_B(\rho(|\psi\rangle\langle\psi|\otimes\mathbb{1}_B))) = \mathrm{Tr}(\rho(|\psi\rangle\langle\psi|\otimes\mathbb{1}_B)). \quad (14)$$

It is easy to see that the latter must be positive. For this consider the spectral decomposition of $\rho = \sum_i \lambda_i|\psi_i\rangle\langle\psi_i|$. We moreover use the decomposition $\mathbb{1}_B = \sum_{j=1}^{d_B}|j\rangle\langle j|$ The latter then yields

$$\mathrm{Tr}(\rho(|\psi\rangle\langle\psi| \otimes \mathbb{1}_B)) = \sum_{i,j}\lambda_i \mathrm{Tr}(|\psi_i, j\rangle\langle\psi_i, j||\psi\rangle\langle\psi|) = \sum_{i,j}\lambda_i|\langle\psi_i, j|\psi\rangle|^2. \quad (15)$$

As all λ_i are positive, the latter is a sum over positive numbers and hence positive.

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

$$\mathrm{Tr}(\rho_{AB}O_A \otimes \mathbb{1}_B) = \mathrm{Tr}(\mathrm{Tr}_B(\rho_{AB})O_A). \quad (16)$$

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

Solution: We show this for all matrices ρ_{AB} of the form $M_A \otimes N_B$. We have

$$\mathrm{Tr}(M_A \otimes N_B(O_A \otimes \mathbb{1}_B)) = \mathrm{Tr}(M_AO_A \otimes N_B) = \mathrm{Tr}(M_AO_A)\mathrm{Tr}(N_B), \quad (17)$$

which also equals the right hand side of (16). The claim follows from the fact that trace and partial trace are linear and that matrices of the form $M_A \otimes N_B$ span the vector space of all matrices.

g) Reduced states of pure states are not necessarily pure. Let $d_A = d_B =: d$. Show that there is in fact no pure state $|\psi_A\rangle\langle\psi_A|$ acting on A that satisfies (16) 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*.

Solution: We can simply choose an observable O_A that violates (16). In particular, we choose $O_A = |\phi\rangle\langle\phi|$, where $|i\rangle$ is an arbitrary basis state in $\mathbb{C}^{d_A}$. However, we have that (16) always implies

$$\mathrm{Tr}(\rho_{AB} O_A \otimes \mathbb{1}) = \mathrm{Tr}(|\phi\rangle\langle\phi|\mathbb{1}_A/d_A) = 1/d_A. \tag{18}$$

but for a pure state $|\psi_A\rangle\langle\psi_A|$ we have for the right hand side of (16)

$$\mathrm{Tr}(|\psi_A\rangle\langle\psi_A|\phi\rangle\langle\phi|) = |\langle\phi|\psi_A\rangle|^2. \tag{19}$$

Clearly this can not be $1/d_A$ for all choices of $|\phi\rangle$.

2. **An example**
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.

   Solution: The state $\rho_1 = |\psi\rangle\langle\psi|$ with $\psi = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is a pure state, while ρ_2 is not because $\mathrm{Tr}(\rho_2^2) = \frac{1}{4}\mathrm{Tr}(\mathbb{1}^2) = \frac{1}{2}$.

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

   Solution: We find $\langle Z\rangle_{\rho_1} = 0$, $\langle Z\rangle_{\rho_2} = 0$, $\langle X\rangle_{\rho_1} = 1$ and $\langle X\rangle_{\rho_2} = 0$.

   c) Give an example of a physical system that can be described by $\mathcal{H} = \mathbb{C}^2$ and prescriptions to prepare the states ρ_1 and ρ_2 in this setting. What are the physical observables that correspond to Z and X?

   Solution: The spin degree of freedom of a spin-$1/2$ particle can be described by the Hilber space $\mathbb{C}^2$. We identify the computational basis states $|0\rangle$, $|1\rangle$ with spin aligned and anti-aligned in z-direction, respectively. The state ρ_1 can than be prepared by aligning the spin the particle in x-direction (e.g. by magnetic fields or measuring and post-selection). ρ_2 can be prepared by randomly choosing between preparing spin-up or spin-down photons with probability $\frac{1}{2}$ or just waiting until we completely lost experimental control over the spin degree. The observables σ_z and σ_x correspond to spin in z- and x-direction, respectively.

   Another example would be the polarisation of a single photon, where one for example identifies the computational basis states $|0\rangle$, $|1\rangle$ with horizontal and vertically polarised

3. **Dual space**
On the last sheet, we got familiar with the construction of the tensor product of Hilbert spaces. In this exercise, we will see that tensor product spaces are not only useful to describe multi-partite systems but also come up naturally when considering linear maps on Hilbert spaces.

The dual (vector) space of a vector space $\mathcal{H}$ is defined as $\mathcal{H}^* := \{\langle\psi| : \mathcal{H} \to \mathbb{C}, \text{linear}\}$. $\mathcal{H}^*$ possesses a dual basis $\{\langle i|\}_{i=1}^d$ with respect to B_1 by requiring orthonomality $\langle i|j\rangle = \delta_{ij}$. The dual space is itself a vector space.[1]

[1] Note that the notation to choose "flipped" ket-vectors (bras) for elements in the dual space is a arbitrary choice we make. As we will see in this exercise and you probably know from your introductory QM course, it can make calculations very easy due to the similarity of the dual vector space to the vector space itself, not to mention the obvious similarity of $\langle i|j\rangle$ to the commonly used symbol for the scalar product $\langle i, j\rangle$. Still, one has to keep in mind why this this all works.

a) Define an orthonomal basis of the dual space of $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Solution: Let $\{\langle i|\}_{i=1}^d$ be a orthonomal basis of $\mathcal{H}_1^*$ and $\{\langle j|\}_{j=1}^D$ a basis of $\mathcal{H}_2^*$. The dual basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ can then be labelled by $B_{1,2}^* = \{\langle i,j|\}_{i=1,\dots,d;j=1,\dots,D}$.

b) Equip the dual space with a canonical scalar product and show that it becomes a Hilbert space. (Regarding the completeness, a comment is sufficient.)

Solution: We can use the scalar product on $\mathcal{H}_1^*$ and $\mathcal{H}_2^*$, respectively, to define a scalar product on $(\mathcal{H}_1 \otimes \mathcal{H}_2)^* = \mathcal{H}_1^* \otimes \mathcal{H}_2^*$. In particular, we define $\langle i,j|i',j'\rangle := \langle i|i'\rangle \langle j|j'\rangle = \delta_{i,i'}\delta_{j,j'}$. And two arbitrary elements $\langle a|, \langle b| \in \mathcal{H}_1^* \otimes \mathcal{H}_2^*$ we define it by extending it linearly. Let $\langle a| = \sum_{i=1}^d \sum_{j=1}^D a_{i,j} \langle i,j|$ and $\langle b| = \sum_{i=1}^d \sum_{j=1}^D b_{i,j} \langle i,j|$. We define

$$\begin{aligned}\langle a|b\rangle &:= \sum_{i,i'=1}^d \sum_{j,j'=1}^D a_{i,j} b_{i',j'}^* \langle i,j|i',j'\rangle \\ &= \sum_{i=1}^d \sum_{j=1}^D a_{i,j} b_{i,j}^*.\end{aligned}$$

With this definition we can check the Hilbert space properties easily. Let $\langle a|, \langle b| \in \mathcal{H}_1^* \otimes \mathcal{H}_2^*$.

1. Symmetry: $\langle b|a\rangle = \sum_{i=1}^d \sum_{j=1}^D a_{i,j}^* b_{i,j} = \left(\sum_{i=1}^d \sum_{j=1}^D a_{i,j} b_{i,j}^*\right)^* = (\langle a|b\rangle)^*$, where we used the linearity of complex conjugation.

2. Linearity: Since we have defined the scalar product as a linear extension of the scalar product on the basis (dual) vectors, linearity follows by construction.

3. Positive definiteness: $\langle a|a\rangle = \sum_{i=1}^d \sum_{j=1}^D a_{i,j} a_{i,j}^* = \sum_{i=1}^d \sum_{j=1}^D |a_{i,j}|^2 \geq 0$ and is equal to zero if and only if $a_{i,j} = 0 \forall i,j$ which is only the case for the zero (dual) vector.

4. Completeness: Since the dual space is a **finite dimensional** vector space – just as the non-dual space is – it is guaranteed to be complete with the above scalar product.

We denote the vector space of linear operators on $\mathcal{H}$ by $L(\mathcal{H}) = \{X : \mathcal{H} \to \mathcal{H}, \text{linear}\}$.

c) Show that $L(\mathcal{H})$ is isomorphic to $\mathcal{H} \otimes \mathcal{H}^*$.

Solution: First, note that $L(\mathcal{H})$ is a vector space spanned by the (linear) projectors $\{\pi_{i,j} : \mathcal{H} \to \mathcal{H}, \pi_{i,j}(|k\rangle) = \delta_{j,k}|i\rangle ; i,j,k = 1,\dots,\dim(\mathcal{H})\}$. Note that this definition (action on the basis elements) suffices to define these projectors uniquely. We now just have to find a one-to-one mapping from $\{\pi_{i,j}\}$ to $\mathcal{H}$. The latter space is spanned by $\{|i\rangle \otimes \langle j| =: |i\rangle\langle j| ; i,j = 1,\dots,\dim(\mathcal{H})\}$. The isomorphism is given by $\pi_{i,j} \mapsto |i\rangle\langle j|$. We confirm it by calculating the action of the right hand side on an arbitrary basis vector $|k\rangle$: $(|i\rangle\langle j|)|k\rangle = |i\rangle \langle j|k\rangle = \delta_{j,k}|i\rangle = \pi_{i,j}(|k\rangle)$.

d) Use the isomorphism established in the previous task to define the tensor product $A \otimes B$ of two operators $A, B \in L(\mathcal{H})$.

Solution: Any map in $L(\mathcal{H})$ can be expanded in terms of $\{\pi_{i,j}\}$ and with the isomorphism above, in terms of $\{|i\rangle\langle j|\}$. This gives a natural way to define the tensor product on operators following the procedure above and on the previous sheet. For $A = \sum_{i=1}^{\dim(\mathcal{H})} A_{i,j} |i\rangle\langle j|$ and $B = \sum_{i=1}^{\dim(\mathcal{H})} B_{i,j} |i\rangle\langle j|$, we define

$$\begin{aligned} A \otimes B &:= \sum_{i,j,i',j'=1}^{\dim(\mathcal{H})} A_{i,j} B_{i',j'} |i\rangle\langle j| \otimes |i'\rangle\langle j'| \\ &= \sum_{i,j,i',j'=1}^{\dim(\mathcal{H})} A_{i,j} B_{i',j'} |i,i'\rangle\langle j,j'| \,. \end{aligned}$$

4. **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 (as you will see in the next lecture). Bell inequalities (and their violation by quantum mechanics) capture rigorously the discomfort that Einstein, Podolsky and Rosen (EPR) famously formulate in their 1935 paper, demanding that

> "In a complete theory there is an element corresponding to each element of reality."

In this exercise, we want to investigate theories of the type EPR consider *complete*, namely, *local and realistic* theories.

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 *tests* or measurements on those particles by adjusting their measurement apparatus.

More precisely, Alice and Bob (randomly) choose between two configurations $s \in \mathcal{S} = \{\pm 1\}$ of their measurement apparatus as soon as the particles arrive. The outcomes of their tests A, B may be ± 1 and depend on how Charlie prepares the particles, the details of his apparatus, and so on. All of Charlie's parameters described by some configuration λ in some configuration space Λ as well as the distribution $p(\lambda)$ according to which he picks a configuration are unknown to Alice and Bob, while, of course, their measurement setting is known to them. 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 tests. Consequently, we can assign deterministic functions

$$A, B : \mathcal{S} \times \mathcal{S} \times \Lambda \to \{\pm 1\} \,,$$

  for Alice's and Bob's test, respectively.

- *Locality*: Alice's performing her test (somewhere space-like separated) does not influence the result of Bob's measurement, and vice versa. This implies that in fact the outcome of A, B only depends on the respective test configuration of Alice or Bob so that we can write

$$\begin{aligned} A &: \mathcal{S} \times \Lambda \to \{\pm 1\}; \ (s, \lambda) \mapsto A_s(\lambda) \\ B &: \mathcal{S} \times \Lambda \to \{\pm 1\}; \ (s, \lambda) \mapsto B_s(\lambda) \end{aligned}$$

We will now look at the S-parameter

$$S = \langle A_1 B_1 + A_2 B_1 + A_1 B_2 - A_2 B_2 \rangle_\lambda \tag{20}$$

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) Derive an upper bound on the absolute value of the S-parameter for a local realistic theory of the type described above.

Solution: Observe that

$$\begin{aligned}&\langle A_1B_1 + A_2B_1 + A_1B_2 - A_2B_2\rangle_\lambda \\ &\quad = \sum_\lambda p(\lambda)[(A_1(\lambda) + A_2(\lambda))B_1(\lambda) + (A_1(\lambda) - A_2(\lambda))B_2(\lambda)] \in [-2, 2].\end{aligned}$$

since either the first term or the second term in the sum is 0 and the other one ± 2. Since p is a probability distribution the sum is upper and lower bounded by ± 2, respectively.

Now assume that Charlie does not send an arbitrary pair of particles, but a quantum-mechanical maximally entangled state $|\psi\rangle := (|00\rangle + |11\rangle)/\sqrt{2}$ where the first tensor copy is sent to Alice and the second to Bob. Alice measures either $A_1 = X \otimes \mathbb{1}$ or $A_2 = Z \otimes \mathbb{1}$ on her copy of the state, while Bob measures either $B_1 = \mathbb{1} \otimes (Z + X)/\sqrt{2}$ or $B_2 = \mathbb{1} \otimes (X - Z)/\sqrt{2}$.

b) Calculate S in this setting. What do you conclude?

Solution: We get

$$\frac{1}{\sqrt{2}}\langle\psi|Z \otimes (X - Z)|\psi\rangle = -\frac{1}{\sqrt{2}}$$
$$\frac{1}{\sqrt{2}}\langle\psi|X \otimes (X - Z)|\psi\rangle = \frac{1}{\sqrt{2}}\langle\psi|X \otimes (X + Z)|\psi\rangle = \frac{1}{\sqrt{2}}\langle\psi|Z \otimes (X + Z)|\psi\rangle = \frac{1}{\sqrt{2}}$$

such that $S = 2\sqrt{2}$

This example is an instance of the more general question, what values S can take if the outcomes of tests as above are described by quantum mechanics. In this case, Charlie's configuration space is just the space of quantum states on two copies of a Hilbert space, which we take to be the density matrices on two qubits: $\mathcal{D}(\mathbb{C}^2 \otimes \mathbb{C}^2)$. The tests Alice and Bob are allowed to perform are just two dichotomic measurements (i.e., measurements with outcomes ± 1) each, so $A_i \otimes \mathbb{1}$, and $\mathbb{1} \otimes B_i$, $i = 1, 2$, with $A_i, B_i \in \mathcal{B}(\mathbb{C}^2)$.

We can therefore write the S-parameter as

$$S_{\mathrm{qm}} = \langle A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2\rangle_\rho\,, \tag{21}$$

where $\langle\cdot\rangle_\rho = \mathrm{Tr}[\cdot\,\rho]$ now denotes the quantum-mechanical expectation value.

c) Show that

$$(A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2)^2 = 4\mathbb{1} - [A_1, A_2] \otimes [B_1, B_2]\,, \tag{22}$$

to derive an upper bound on S_{qm}.

Solution: Expand and calculate $X = (A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2)$ using that $A_i^2 = \mathbb{1} = B_i^2$ since both are dichotomic measurements with outcomes ± 1.

We are interested in $S_{\mathrm{qm}} = \langle X\rangle_\rho = \langle\sqrt{X^2}\rangle_\rho$. But then, it is easy to see, using that $X^2 = U\Lambda U^\dagger$ that

$$\langle\sqrt{X^2}\rangle_\rho = \mathrm{Tr}[U\sqrt{\Lambda}U^\dagger\rho] = \mathrm{Tr}[\sqrt{\Lambda}U^\dagger\rho U] \le \max_{\rho' = U^\dagger\rho U} \mathrm{Tr}[\sqrt{\Lambda}\rho'] \tag{23}$$

$$\le \max_{\rho'}\left((\max_i \sqrt{\lambda_i})\sum_i \rho'_{ii}\right) = \max_i \sqrt{\lambda_i}\,. \tag{24}$$

We now observe that $\max_i \sqrt{\lambda_i}$ is the operator norm and use the triangle inequality to arrive at $S_{\mathrm{qm}} \leq \sqrt{8}$. Notice that the operator norms of $\mathbb{1}, A, B$ are 1.

Alternatively, one can directly use the norm bound

$$\langle X \rangle_\rho^2 \leq \|X\|^2 = \|X^2\| \leq 4\|\mathbb{1}\| + 4\|A_1\|\|A_2\|\|B_1\|\|B_2\| = 8\,, \tag{25}$$

where we used the Hölder inequality, submultiplicativity and the triangle inequality.