Quantum information theory (MAT4430) **Spring 2021**

Lecture 3: The theory of open quantum systems

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When encountering a specific quantum system, there are two problems to be solved in order to harness it for quantum information processing:

1. We need to find a description of the system in the quantum mechanical formalism.
2. We need to engineer information theoretic protocols for the system using the quantum mechanical formalism.

In this course, we will exclusively focus on the second problem. We will not describe any particular quantum system, but instead study the capabilities and fundamental limits of general quantum systems to process different kinds of information. To do so, we will need an abstract version of the formalism of quantum theory, which can be seen as an extension of classical probability theory.

1 The big picture

The formalism of quantum mechanics is based on three fundamental notions: *States*, *time-evolutions* and *measurements*. The state of a general physical system describes all its properties, or at least all the properties we care about in some physical description. The formalism of time-evolutions describes how the system evolves in time after being in some initial state. To compute the time-evolution of a system we usually need to know how its constituents interact with each other. In classical physics, we would be done now, but in quantum physics a special role is played by the measurement process. Formally, a measurement is distinct from time-evolutions in two aspects: While the time-evolution in quantum mechanics will turn out to be *reversible*, i.e., the state at some time uniquely determines the state at prior times, this is not true for measurements where the state undergoes an irreversible change. The time-evolution is also *deterministic* in the sense that states at all times are uniquely determined by the states at prior times. However, measurements are fundamentally probabilistic, i.e., random measurement outcomes will be observed with a probability distribution determined by the measurement and the state that is measured. The problem to reconcile these two conflicting descriptions of reality is called the *measurement problem*. To this day, it is an open problem at the foundation of quantum mechanics. While the strange predictions of quantum theory have been replicated in experiments countless times to high degrees of accuracy we are far away from resolving this issue.

On the way to a general formalism of quantum mechanics, we will start by the description of *closed* quantum systems. A quantum system is called *closed* when it does not interact with any other quantum system. Historically, this was the starting point for quantum theory, but it was later observed that this description is unsatisfactory: Even in well-controlled labratory settings, quantum systems will interact with the environment (e.g., through magnetic fields from electric currents, radioactive background or cosmic radiation) and can therefore not considered to be closed. In principle, we could consider the whole universe as a closed quantum system, but this would be hopelessly complicated. Instead, we will develop a general formalism of *open* quantum systems, i.e., quantum systems that may interact with an environment, which include the closed quantum systems as a special case. This will lead to the general formalism commonly used in quantum information theory and throughout the rest of the course.

2 The first postulate: State space

The formalism of quantum mechanics in its modern form is build upon the theory of Hilbert spaces, or complex Euclidean spaces if we restrict to finite dimensions. In this course, we will restrict to finite-dimensional quantum systems and measurements with finitely many outcomes. In practice, this is usually no restriction since any experiment will only have a finite resolution and therefore all occurring objects can be discretized accordingly.

Postulate 1 (State space)**.** *For every quantum system, there is an associated complex Euclidean space $\mathcal{H}$ called the* state space*.*

The first postulate sets the stage for the general formalism and we will have to explain how to model states, time-evolutions and measurements on general state spaces.

3 Postulates for closed quantum systems

Let us start with the postulates of quantum mechanics for closed quantum systems. In this section, $\mathcal{H}$ will always denote the state space of the closed system.

Postulate 2 (Pure states)**.** *The states of a closed quantum system are represented by vectors $|\psi\rangle \in \mathcal{H}$ satisfying $\langle\psi|\psi\rangle = 1$.*

As we will see below, the previous postulate is not entirely true: While every state of a closed system can be represented by a normalized vector in Hilbert space, this representation is redundant. This aspect is crucial, and we will discuss it further towards the end of this section.

Postulate 3 (Time-evolution of closed systems)**.** *Interaction within the system is modelled via a Hermitian operator $H \in B(\mathcal{H})_{sa}$ called the* Hamiltonian*. When the system is initially prepared in a pure state $|\psi\rangle \in \mathcal{H}$, then the time-evolution is described by the* Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = iH|\psi(t)\rangle, \quad |\psi(0)\rangle = |\psi\rangle.$$

Let us pause for a while, to fully appreciate the previous postulate. For any Hamiltonian $H \in B(\mathcal{H})_{sa}$ the Schrödinger equation can be solved by defining the evolution operator $U_t : \mathcal{H} \to \mathcal{H}$ by $U_t = \exp(iHt)$ for each $t \in \mathbb{R}$. For an initial state $|\psi(0)\rangle = |\psi\rangle \in \mathcal{H}$, the time-evolution is then described by

$$|\psi(t)\rangle = U_t|\psi\rangle.$$

It is easy to check, that $\{U_t\}_{t\in\mathbb{R}}$ defines a group of unitary operators with identity $U_0 = \mathbb{1}_{\mathcal{H}}$ and $U_t^{-1} = U_{-t}$. In fact, we have the easy describtion $U_t = U^t$ for the fixed unitary $U = \exp(iH)$. Postulate 3 implies that closed quantum systems evolve by a unitary transformation. Moreover, for any given unitary $U \in \mathcal{U}(\mathcal{H})$, we can always find a Hamiltonian $H \in B(\mathcal{H})_{sa}$ such that $U = \exp(iH)$ and therefore, we can formulate the previous postulate in the following alternative form:

Postulate 3′ (Time-evolution of closed systems II)**.** *If the closed system is in an inital state $|\psi\rangle \in \mathcal{H}$ and evolves in time to a state $|\psi'\rangle \in \mathcal{H}$, then there exists a unitary operator $U \in \mathcal{U}(\mathcal{H})$ such that $|\psi'\rangle = U|\psi\rangle$.*

Finally, we need to introduce the notion of measurement. Note that measurements require an interaction of the closed system with an external observer, and strictly speaking this means that our quantum system is no longer closed when this happens. In this sense, the system does not need to evolve according to a unitary transformation during the measurement process, and indeed we will see that (in general) it does not. In fact, the measurement process will result in an instantaneous and irreversible change of the system's state, which has been referred to as the collaps of the wave function.

Postulate 4 (Projection-valued measure (PVM))**.** *For every measurement of a closed quantum system there is an associated set of projections* $\{P_n\}_{n=1}^N \subset \mathrm{Proj}\,(\mathcal{H})$ *corresponding to measurement outcomes* $n \in \{1, \ldots, N\}$ *and satisfying* $\sum_{n=1}^N P_i = \mathbb{1}_{\mathcal{H}}$*. Measuring a state* $|\psi\rangle \in \mathcal{H}$ *results in the outcome* n *with probability*

$$p_n = \langle\psi|P_n|\psi\rangle.$$

After measuring a state $|\psi\rangle \in \mathcal{H}$ *and obtaining the outcome* n*, the system is in the post-measurement state*

$$|\psi_n\rangle = \frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}.$$

Measurements are the only way to obtain classical data from a quantum state. Since any measurement is a probabilistic process, we will usually consider the whole statistics of measurement outcomes as the classical data obtained from the measurement. Here, it is tacitly assumed that we can perform some sort of experiment (see Figure 1), consisting of a preparation of the state and a measurement, many times independently to obtain the statistics of outcomes. This can be seen as the most basic *interpretation* of quantum mechanics, saying that the mathematical objects are just describing the statistics obtained from repeating identitcal experiments and nothing more. However, there are other interpretations and the question whether the quantum states should be considered as "real" or just as "states of knowledge" is the subject of ongoing debate. Another major problem at the foundation of quantum theory is the measurement problem:

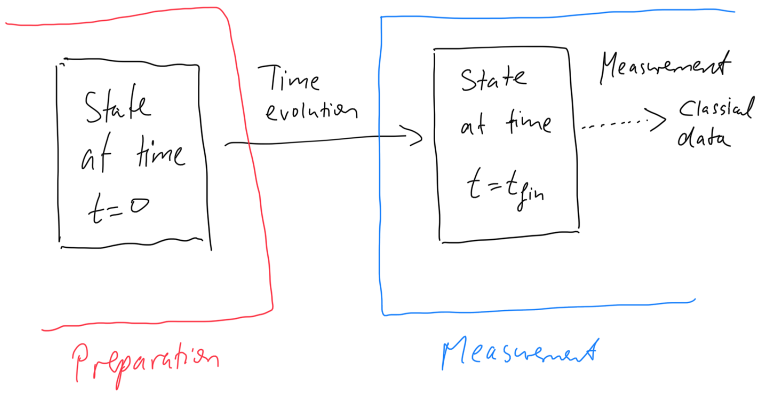

Figure 1: A quantum experiment.

Problem 3.1 (The measurement problem)**.** *What is the physical process behind the measurement formalism? How can it change the state of the system instantly? Why is this process formally different to a time-evolution, when every measurement apparatus should, in principle, also be a quantum system?*

We need to make some further remarks about PVM defined in the Postulate 4. It can be shown that the projection operators in any PVM are orthogonal, i.e., they satisfy $P_n P_m = 0$ whenever $n \neq m$. This has an important consequence: After measuring the system and obtaining an outcome $n \in \{1, \ldots, N\}$ measuring the system again will always result in the same outcome n. It can therefore be said, that the system's state does not have a well-defined ("classical") value of the quantity measured by a PVM prior to the measurement process, but that afterwards the value is well-defined.

Postulate 4 has an important implication for our version of Postulate 2 stated above: Note that the probabilities $p_n = \langle\psi|P_n|\psi\rangle$ of obtaining the outcome $n \in \{1, \ldots, N\}$ are the same when measuring any state $e^{i\alpha}|\psi\rangle \in \mathcal{H}$ for $\alpha \in \mathbb{R}$ with the PVM $\{P_n\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H})$. We say that the measurement statistics does not depend on any *global phase factor*. Since measurement outcomes are all the information we can ever obtain from a quantum system it makes sense to identify all vectors $e^{i\alpha}|\psi\rangle \in \mathcal{H}$ and refer to them as a single state. Formally, this means that we should consider pure states as elements of a complex projective space. There is a simple an elegant solution to this problem, which we will adopt in the general formalism. Instead of representing pure states by vectors $|\psi\rangle \in \mathcal{H}$, we will represent them by rank-1 projections $|\psi\rangle\langle\psi| \in \mathrm{Proj}(\mathcal{H})$. Note that this takes care of the aforementioned issue and all vectors $e^{i\alpha}|\psi\rangle$ for $\alpha \in \mathbb{R}$ and some fixed $|\psi\rangle \in \mathcal{H}$ define the same projector $|\psi\rangle\langle\psi|$. Moreover, we can formulate all the previous postulates by using projections instead:

- **Pure states:** Every state of a closed system is represented by a projection $|\psi\rangle\langle\psi| \in \mathrm{Proj}(\mathcal{H})$ for some $|\psi\rangle \in \mathcal{H}$.

- **Time-evolution:** States of closed systems evolve unitarily, i.e., $|\psi\rangle\langle\psi| \mapsto U|\psi\rangle\langle\psi|U^\dagger$ for some unitary $U \in \mathcal{U}(\mathcal{H})$.

- **Measurements:** Measuring a pure state $|\psi\rangle\langle\psi| \in \mathrm{Proj}(\mathcal{H})$ using a PVM $\{P_n\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H})$ results in measurement outcome $n \in \{1, \ldots, N\}$ with probability

  $$p_n = \langle\psi|P_n|\psi\rangle = \mathrm{Tr}\left[|\psi\rangle\langle\psi|P_n\right].$$

  After obtaining the outcome $n \in \{1, \ldots, N\}$, the system is in the state

  $$|\psi_n\rangle\langle\psi_n| = \frac{P_n|\psi\rangle\langle\psi|P_n}{\langle\psi|P_n|\psi\rangle}.$$

So far, we have only considered a single closed quantum system without any additional structure. In quantum information theory, we will often encounter quantum systems that are composed of simpler systems. The last postulate describes the state space of such compositions:

Postulate 5 (Composite systems)**.** *If a closed quantum system is composed of two quantum systems with state spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, then its state space is given by the tensor product $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$.*

This postulate has profound consequences for the description of quantum systems. For example, it implies that the dimension of the state space of a quantum system composed of N quantum systems with d-dimensional state spaces is d^N, i.e., exponentially large in the number N. This fact makes it very challenging to numerically simulate quantum systems on classical computers and it is one motivation to develop quantum computers which could simulate quantum systems faster.

Let us close this section with an important observation: There are two distinct classes of pure states on composite systems:

- **Pure product states:** These are states of the form $|\psi_{AB}\rangle\langle\psi_{AB}| = |\phi_A\rangle\langle\phi_A| \otimes |\tau_B\rangle\langle\tau_B|$ for pure states $|\phi_A\rangle\langle\phi_A| \in \mathrm{Proj}(\mathcal{H}_A)$ and $|\tau_B\rangle\langle\tau_B| \in \mathrm{Proj}(\mathcal{H}_B)$.

- **Pure entangled states:** These are states of the form $|\psi_{AB}\rangle\langle\psi_{AB}| \in \mathrm{Proj}(\mathcal{H}_A \otimes \mathcal{H}_B)$ that are not pure product states.

In the next section, we will obtain a description for the state of a system 'A' that is part of a closed composite system 'AB' in some pure state $|\psi_{AB}\rangle\langle\psi_{AB}|$. If the composite system 'AB' is in a product pure state $|\psi_{AB}\rangle\langle\psi_{AB}| = |\phi_A\rangle\langle\phi_A| \otimes |\tau_B\rangle\langle\tau_B|$, then this is quite easy, and we should just take the pure state $|\phi_A\rangle\langle\phi_A|$ to be the state of the system 'A'. Why does this make sense? Consider the situation, where you have two closed quantum systems 'A' and 'B' modelled by the complex Euclidean spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. The formalism of closed quantum systems can then be applied in the following way (see Figure 2):

- **Pure states of a pair of closed systems:** Pure product states

$$|\psi_{AB}\rangle\langle\psi_{AB}| = |\phi_A\rangle\langle\phi_A| \otimes |\tau_B\rangle\langle\tau_B|.$$

- **Product time-evolution:** Time-evolution by product unitary $U_A \otimes U_B$ for $U_A \in \mathcal{U}(\mathcal{H}_A)$ and $U_B \in \mathcal{U}(\mathcal{H}_B)$.
- **Product measurement:** The measurement using the product PVM $\{P_n^A \otimes P_m^B\}_{n,m}$ for PVMs $\{P_n^A\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H}_A)$ and $\{P_n^B\}_{m=1}^M \subset \mathrm{Proj}(\mathcal{H}_B)$.

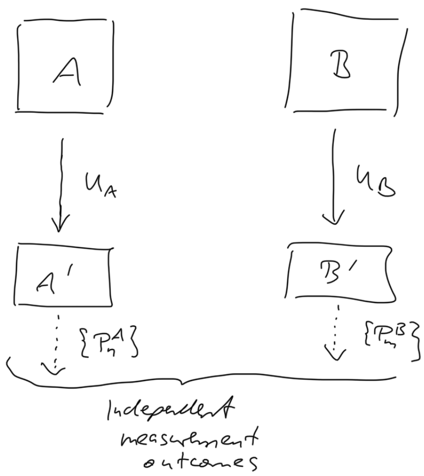

Figure 2: Two closed quantum systems.

Note that measuring a pure product state $|\phi_A\rangle\langle\phi_A| \otimes |\tau_B\rangle\langle\tau_B|$ using a product measurement $\{P_n^A \otimes P_m^B\}_{n,m}$ yields the product distribution $p_A \times p_B$ of the outcome distributions p_A and p_B obtained from measuring the pure states $|\phi_A\rangle\langle\phi_A|$ and $|\tau_B\rangle\langle\tau_B|$ with the PVMs $\{P_n^A\}_{n=1}^N$ and $\{P_n^B\}_{m=1}^M$, respectively. This is exactly, what we should expect from measuring two closed systems, which, by definition, do not interact with each other or any other system. Evolving the systems using product time-evolutions only leads to other product states, and the closedness of the systems is preserved.

4 Quantum states

What is the problem with the formalism of closed quantum systems? Consider the situation where you want to describe a quantum system contained in your laboratory, which is affected by the environment outside of the laboratory. An example could be an atom that is affected by the electromagnetic field of a nearby powerline, or by cosmic radiation coming from particles crashing into earth's atmosphere at high speed. It seems hopeless to describe the closed system consisting of the lab, and all other quantum systems that might interact with

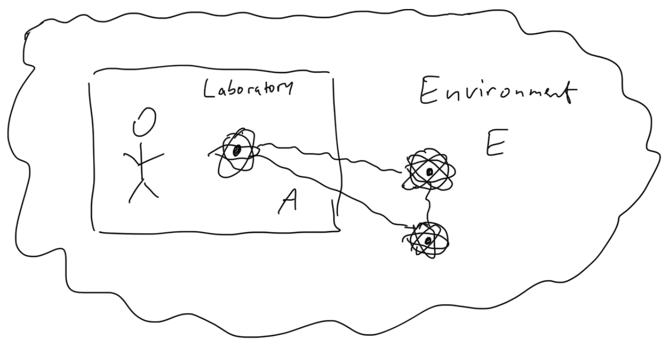

Figure 3: The laboratory as an open quantum system.

it. The *formalism of open quantum systems* solves this problem and it allows us to treat the system of interest directly.

The philosophy behind this approach assumes the universe to be split in two parts: The system 'A' we are interested in (e.g., the laboratory which we can control) and the environment 'E' which interacts with our system in a complicated way (and which we cannot control!). See Figure 3 for a visualization. Together the composite system 'AE' will be closed and we can use the postulates of closed quantum systems to describe its pure states, time-evolutions and measurements. The formalism we are going to develop allows us to express these objects on the system 'A' alone, which amounts to treat 'A' as an open quantum system (being part of the system 'AE' joint with the environment). The notion of *density operators* is at the basis of this formalism. We will simply call these objects *quantum states*, since they generalize pure quantum states, and in the following we will see how they arise naturally from the formalism of closed quantum systems.

Quantum states from quantum marginals: Given a composite quantum system, how can we talk about the subsystems individually? How should we represent their state? We can use the measurement formalism to answer this question. Imagine a setting, where there are two systems 'A' and 'E' modelled by complex Euclidean spaces $\mathcal{H}_A$ and $\mathcal{H}_E$, respectively, such that their composition 'AE' is closed. Given a PVM $\{P_n\}_{n=1}^N \subset \mathrm{Proj}\,(\mathcal{H}_A)$, we aim to find a PVM $\{Q_n^{AE}\}_{n=1}^N \subset \mathrm{Proj}\,(\mathcal{H}_A \otimes \mathcal{H}_E)$ that describes the measurement process when measuring the PVM $\{P_n\}_{n=1}^N$ on the system 'A' alone. A reasonable guess would be to set

$$Q_n^{AE} = P_n \otimes \mathbb{1}_{\mathcal{H}_E}, \tag{1}$$

for every $n \in \{1, \ldots, n\}$. We will now show that there is no other choice for this PVM:

Theorem 4.1. *The PVM $\{Q_n^{AE}\}_{n=1}^N \subset \mathrm{Proj}\,(\mathcal{H}_A \otimes \mathcal{H}_E)$ given by* (1) *is the only PVM for which the outcome distribution when measuring the pure product state $|\phi_A\rangle\langle\phi_A| \otimes |\tau_B\rangle\langle\tau_B|$ for any $|\phi_A\rangle\langle\phi_A| \in \mathrm{Proj}\,(\mathcal{H}_A)$ and any $|\tau_B\rangle\langle\tau_B| \in \mathrm{Proj}\,(\mathcal{H}_B)$ coincides with the outcome distribution of measuring the pure state $|\phi_A\rangle\langle\phi_A|$ with the PVM $\{P_n\}_{n=1}^N$.*

Proof. Consider the pure states

$$|\psi_{AE}^{(n)}\rangle\langle\psi_{AE}^{(n)}| = \frac{P_n|\phi_A\rangle\langle\phi_A|P_n}{\langle\phi_A|P_n|\phi_A\rangle} \otimes |\tau_E\rangle\langle\tau_E|,$$

for any $n \in \{1, \ldots, N\}$, pure states $|\tau_E\rangle\langle\tau_E| \in \mathrm{Proj}\,(\mathcal{H}_E)$ and $|\phi_A\rangle\langle\phi_A| \in \mathrm{Proj}\,(\mathcal{H}_A)$. In each of these states, the 'A' system is in a post-measurement state of the PVM $\{P_n\}_{n=1}^N \subset \mathrm{Proj}\,(\mathcal{H}_A)$ and we know that another measurement with the same PVM leads to a deterministic outcome. By the assumptions on $\{Q_n^{AE}\}_{n=1}^N \subset \mathrm{Proj}\,(\mathcal{H}_A \otimes \mathcal{H}_E)$ we have

$$\mathrm{Tr}\left[\left(P_n|\phi_A\rangle\langle\phi_A|P_n \otimes |\tau_E\rangle\langle\tau_E|\right) Q_m^{AE}\right] = \langle\phi_A|P_n|\phi_A\rangle\delta_{nm}, \tag{2}$$

for each $n, m \in \{1, \dots, N\}$ and any pure states $|\tau_E\rangle\langle\tau_E| \in \mathrm{Proj}(\mathcal{H}_E)$ and $|\phi_A\rangle\langle\phi_A| \in \mathrm{Proj}(\mathcal{H}_A)$. Defining the positive operator

$$Q_m^A[\tau_E] = (\mathbb{1}_A \otimes \langle\tau_E|)\, Q_m^{AE}\, (\mathbb{1}_A \otimes |\tau_E\rangle),$$

we conclude that

$$\langle\phi_A|P_n Q_m^A[\tau_E]\, P_n|\phi_A\rangle = \mathrm{Tr}\left[P_n|\phi_A\rangle\langle\phi_A|P_n Q_m^A[\tau_E]\right] = \langle\phi_A|P_n|\phi_A\rangle\delta_{nm}$$

for each $n, m \in \{1, \dots, N\}$ and any pure state $|\phi_A\rangle\langle\phi_A| \in \mathrm{Proj}(\mathcal{H}_A)$. Since $P_m Q_m^A[\tau_E]\, P_m$ and P_m are selfadjoint operators, we have

$$P_m Q_m^A[\tau_E]\, P_m = P_m.$$

Moreover, we have $\langle\phi_A|P_n Q_m^A[\tau_E]\, P_n|\phi_A\rangle = 0$ whenever $n \neq m$, and using that $Q_m^A[\tau_E]$ is positive, this implies

$$P_n|\phi_A\rangle \in \ker\left(Q_m^A[\tau_E]\right),$$

for any $|\phi_A\rangle \in \mathcal{H}_A$. Since all involved operators are selfadjoint, we conclude that

$$Q_m^A[\tau_E]\, P_n = P_n Q_m^A[\tau_E] = 0,$$

whenever $n \neq m$. Finally, using $\mathbb{1}_{\mathcal{H}_A} - P_m = \sum_{n\neq m} P_n$ shows that

$$Q_m^A[\tau_E]\,(\mathbb{1}_{\mathcal{H}_A} - P_m) = (\mathbb{1}_{\mathcal{H}_A} - P_m)\, Q_m^A[\tau_E] = 0,$$

and since $P_m Q_m^A[\tau_E]\, P_m = P_m$, we find that

$$Q_m^A[\tau_E] = (P_m + (\mathbb{1}_{\mathcal{H}_A} - P_m))\, Q_m^A[\tau_E]\,(P_m + (\mathbb{1}_{\mathcal{H}_A} - P_m)) = P_m,$$

for any $m \in \{1, \dots, N\}$. This identity holds independently of $|\tau_E\rangle \in \mathcal{H}_E$, and it is easy to show (e.g., by expanding it in a basis) that this implies

$$Q_m^{AE} = P_m \otimes \mathbb{1}_{\mathcal{H}_E},$$

for any $m \in \{1, \dots, N\}$, and we are done.

□

The previous theorem implies that the measurement from (1) is the only sensible choice for a PVM corresponding to the partial measurement of $\{P_n\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H}_A)$ on the system 'A' of a joint closed system 'AE'. Of course, it might not be clear that there has to be such a PVM, and in the end it is a physical statement that the measurement formalism extends independently of the underlying state. We will not bother to much about this now, and we just take (1) as the definition of a partial measurement on *any* closed quantum system, i.e., not neccessarily closed quantum systems which are composed of closed quantum systems.

Now, we can get back to our initial question: How can we represent the state of a subsystem of a composite system? For this, consider a PVM $\{P_n\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H}_A)$. If the system 'AE' is in the pure state $|\psi_{AE}\rangle\langle\psi_{AE}| \in \mathrm{Proj}(\mathcal{H}_A \otimes \mathcal{H}_E)$, then measuring the PVM $\{P_n \otimes \mathbb{1}_{\mathcal{H}_E}\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H}_A \otimes \mathcal{H}_E)$ gives outcome n with probability

$$p_n = \mathrm{Tr}\left[|\psi_{AE}\rangle\langle\psi_{AE}|\,(P_n \otimes \mathbb{1}_{\mathcal{H}_E})\right] = \mathrm{Tr}\left[\rho_A P_n\right], \tag{3}$$

where we have introduced the operator

$$\rho_A = (\mathrm{id}_A \otimes \mathrm{Tr})\,(|\psi_{AE}\rangle\langle\psi_{AE}|) := \sum_{i=1}^{d_E} (\mathbb{1}_A \otimes \langle i_E|)\, |\psi_{AE}\rangle\langle\psi_{AE}|\, (\mathbb{1}_A \otimes |i_E\rangle),$$

obtained by applying the trace partially to the pure state $|\psi_{AE}\rangle\langle\psi_{AE}|$. It can be checked that the operator ρ_A is positive and has unit trace. Conveniently, these properties guarantee that the numbers $p_n = \mathrm{Tr}[\rho_A P_n]$ define a probability distribution for any projective measurement $\{P_n\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H}_A)$. Operators with these properties are sometimes called *density operators*, but we will use the following terminology:

Definition 4.2 (Quantum states). *A* quantum state *on $\mathcal{H}$ is a positive operator $\rho \in B(\mathcal{H})^+$ satisfying $\mathrm{Tr}[\rho] = 1$. We denote the set of quantum states by $\mathcal{D}(\mathcal{H})$*

The above reasoning suggests, that ρ_A is the correct object to represent the state of the subsystem 'A' within the composite system 'AE'. Let us state the following definition:

Definition 4.3 (Partial trace). *The linear map $\mathrm{Tr}_B = \mathrm{id}_A \otimes \mathrm{Tr} : B(\mathcal{H}_A \otimes \mathcal{H}_B) \to B(\mathcal{H}_A)$ is called the* partial trace *(on the system 'B'). When no confusion can arise, we will use the notation $\mathrm{Tr}_A, \mathrm{Tr}_B, \mathrm{Tr}_{AB}$, etc., to denote the partial traces for subsystems carrying the corresponding labels.*

The partial trace is analogous to taking the marginal of a classical probability distribution (see Lecture 1). The particular operators ρ_A or ρ_E obtained by taking the partial traces of a pure state $|\psi_{AE}\rangle\langle\psi_{AE}|$ are also known as the *reduced density operators* of $|\psi_{AE}\rangle\langle\psi_{AE}|$. The formalism of open quantum systems will express all measurements and time evolutions in terms of such reduced density operators on the system 'A', i.e., tracing out the environment 'E'. We will later see, that this is equivalent to considering the full set $\mathcal{D}(\mathcal{H})$ of quantum states, i.e., every quantum state arises as the reduced density operator of some pure state.

Quantum states from ensembles: We have seen how quantum states arise naturally as reduced density operators, but there is another natural way of thinking about them. Consider a closed quantum system with associated Euclidean space $\mathcal{H}$ and imagine that we can prepare it in any pure state from a set $\{|\psi_k\rangle\langle\psi_k|\}_{k=1}^K$. Intuitively, it should then be possible to prepare the system in a statistical mixture of pure states, where we prepare the state $|\psi_k\rangle\langle\psi_k|$ with probability q_k for some probability distribution $q \in \mathcal{P}(\{1, \dots, K\})$. How can we represent such a statistical mixture using the Euclidean space $\mathcal{H}$?

Remember that everything we can know about the quantum system is obtained by measurements. What statistics should we expect by measuring our statistical mixture of quantum states using the PVM $\{P_n\}_{n=1}^N \subset \mathrm{Proj}(\mathcal{H})$. By combining the preparation and the measurement we should obtain the measurement outcome n with probability

$$p_n = \sum_{k=1}^K q_k \langle\psi_k|P_n|\psi_k\rangle = \mathrm{Tr}\left[\sum_{k=1}^K q_k |\psi_k\rangle\langle\psi_k| P_n\right]. \tag{4}$$

The previous formula is suggests that we could represent the statistical mixture of the pure states $|\psi_k\rangle\langle\psi_k|$ with probability q_k by the operator

$$\rho = \sum_{k=1}^K q_k |\psi_k\rangle\langle\psi_k|.$$

Again, this operator is *positive* and has *unit trace*, i.e., it is a quantum state. From the spectral theorem, we conclude that each quantum state can be written as some statistical mixture of (orthogonal) pure quantum states. In fact, there are in general many different ways of expressing a density operator as a statistical mixture, and we will see later that it is a crucial property of quantum theory that we cannot tell such equivalent mixtures apart.

It should not come as too much of a surprise that quantum states describe statistical mixtures, since this is a special case of the reduced density matrix from the last chapter. If we consider the quantum state

$$\rho_{CA} = \sum_{k=1}^K q_k |k\rangle\langle k| \otimes |\psi_k\rangle\langle\psi_k|, \tag{5}$$

then we obtain the reduced density operator $\rho_A = \mathrm{Tr}_C[\rho_{CA}] = \sum_{k=1}^K q_k |\psi_k\rangle\langle\psi_k|$.

Quantum states, knowledge and entanglement: There is another point to make reduced density operators and statistical mixtures. How can we tell whether a pure quantum state $|\psi_{AB}\rangle\langle\psi_{AB}|$ is entangled or not? Using the partial trace, this is easy: A pure quantum state $|\psi_{AB}\rangle\langle\psi_{AB}|$ is a product state if and only if its partial trace $\rho_A = \mathrm{Tr}_B\left[|\psi_{AB}\rangle\langle\psi_{AB}|\right]$ is a pure state as well. This fact has an interesting interpretation: Since non-pure density operators arise as statistical mixtures of pure states, they represent situations where our knowledge about the quantum system is incomplete[1] (we do not know which of the pure states has been prepared). In this sense, closed quantum system is in an entangled pure state if and only if our knowledge about its subsystems is incomplete.

5 Time-evolutions of open systems: Quantum channels

How can we model time-evolutions on the quantum system 'A' without having access to the environment 'E'? To answer this question, we will first consider a general, but also very concrete scenario where we can derive the answer from the formalism of closed systems. Afterwards, we will reason more abstractly about these time evolutions and finish this section with a definition.

Concrete quantum channels: Consider first the situation, where the composite system 'AE' is in any pure quantum state $|\psi_{AE}\rangle\langle\psi_{AE}| \in \mathrm{Proj}\left(\mathcal{H}_A \otimes \mathcal{H}_B\right)$ with reduced density operator $\rho_A = \mathrm{Tr}_E\left[|\psi_{AE}\rangle\langle\psi_{AE}|\right]$. If the composite quantum system 'AE' undergoes a time-evolution represented by a unitary operator U_{AE}, then the evolved reduced quantum state is

$$\rho'_A = \mathrm{Tr}_E\left[U_{AE}|\psi_{AE}\rangle\langle\psi_{AE}|U_{AE}^\dagger\right].$$

By computing some examples, it is easy to verify that the map $\rho_A \mapsto \rho'_A$ is not well-defined on reduced density matrices and in general it depends on the pure state $|\psi_{AE}\rangle\langle\psi_{AE}|$ realizing ρ_A as a reduced density operator. This means, that there is no reduced description of this time-evolution, and it can only be described on the whole system 'AE'.

Which time-evolutions can be described on the system 'A' alone? Consider the situation, where the composite system 'AE' is initially in a product quantum state $\rho_A \otimes \sigma_E \in D\left(\mathcal{H}_A \otimes \mathcal{H}_E\right)$ for a fixed quantum state $\sigma_E \in D\left(\mathcal{H}_E\right)$ (not neccessarily pure). Then, the same process as before leads to the well-defined linear map

$$\rho_A \mapsto \rho'_A = \mathrm{Tr}_E\left[U_{AE}\left(\rho_A \otimes \sigma_E\right)U_{AE}^\dagger\right]. \tag{6}$$

While time-evolutions should correspond to transformation of a system 'A', we could also describe general physical processes transforming a system 'A' into another system 'B'. For example, we could consider the situation, where the composite system 'ABE' is in the quantum state $\rho_A \otimes \sigma_{BE}$ for a fixed quantum state $\sigma_{BE} \in D\left(\mathcal{H}_B \otimes \mathcal{H}_E\right)$ (not neccessarily a product state). Using a unitary $U_{ABE} \in \mathcal{U}\left(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_E\right)$, we can obtain a well-defined linear map by

$$\rho_A \mapsto \mathrm{Tr}_{AE}\left[U_{ABE}\left(\rho_A \otimes \sigma_{BE}\right)U_{ABE}^\dagger\right] \in D\left(\mathcal{H}_B\right). \tag{7}$$

The linear maps in (6) and (7) are instances of *quantum channels*, which are the most general physical processes transforming a system 'A' into itself or into a system 'B' definable on the reduced description of these systems alone. Moreover, we will later show that any general quantum channel (see definition below) can be written as in (7) with suitable choices of σ_{BE} and U_{ABE}. Note that, unlike unitary time-evolutions, quantum channels are in general not reversible. Physically, the information needed to reverse the evolution is leaked to the environment and it cannot be reversed on its output alone.

[1]Note that having complete knowledge about a quantum system (i.e, it is in a pure state) does not mean that we can predict measurement outcomes with certainty!

Abstract quantum channels: Let us think more abstractly about physical processes transforming an open system 'A' to an open system 'B'. How should we model such a process? If we can build a formalism based on the notion of quantum states, then physical processes in this formalism should be represented by maps taking quantum states on the input system to quantum states on the output system. Moreover, we should expect such maps to be linear since the time-evolutions on closed quantum systems are linear[2]. Finally, these maps should be applicable to subsystems of larger systems as well. Using the measurement formalism one can again argue, that applying a linear map $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$ partially on the subsystem 'A' of a composite system with Euclidean space $\mathcal{H}_E \otimes \mathcal{H}_A$ amounts to applying the $\mathrm{id}_E \otimes T$. Again, this map should map quantum states to quantum states.

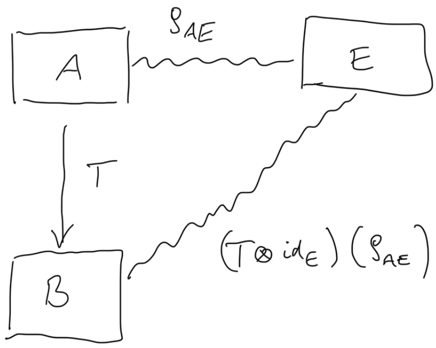

Figure 4: Partial application of a quantum channel.

Let us now properly define the general notions used to formalize quantum theory. We start by introducing some abstract properties of linear maps, which will be crucial in the formalism of open quantum systems. A linear map $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$ is called

- **positive** if $T(X) \in B(\mathcal{H}_B)^+$ for every $X \in B(\mathcal{H}_A)^+$.
- **completely positive** if $(\mathrm{id}_E \otimes T) : B(\mathcal{H}_E) \otimes B(\mathcal{H}_A) \to B(\mathcal{H}_E) \otimes B(\mathcal{H}_B)$ is positive for every complex Euclidean space $\mathcal{H}_E$.
- **trace-preserving** if $\mathrm{Tr}[T(X)] = \mathrm{Tr}[X]$ for every $X \in B(\mathcal{H}_A)$.

Note that every completely positive map is also positive since we can choose $\mathcal{H}_C$ to be 1-dimensional. It can be checked, that the concrete examples of quantum channels in (6) and (7) are completely positive and trace-preserving, and we will take these properties as the basis for a general definition.

Definition 5.1 (Quantum channels)**.** *A linear map* $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$ *is called a* quantum channel *if it is completely positive and trace-preserving.*

6 Measurements of open systems: POVMs and instruments

How should we model measurements of an open quantum system? To answer this question, we will again consider a concrete measurement setting in the formalism of closed quantum systems. Formally, we have to distinguish to problems:

1. What is the most general way to obtain a classical measurement statistics from a quantum system?
2. How does a general measurement process change the state of a quantum system?

[2] For a better argument see...

We will see that these two questions have slightly unrelated answers. We will answer the first question by stating the most general form of *destructive measurements*, i.e., measurements for which the measured quantum system is (considered to be) destroyed in the process. The answer to the second question will lead to a general formalism of *non-destructive measurements*, which contains the destructive measurements as a special case. While it is tempting to focus on the non-destructive case, it is not advised to do so. In many situations the destructive measurement formalism is sufficient and much easier to handle than the non-destructive formalism. Moreover, when we are anyway only interested in classical information about quantum systems, then there is no need to keep any quantum systems indefinitely.

Destructive measurements: In the same way as we have obtained quantum channels as reductions of certain time-evolutions of the composite system 'AE', we can also consider the reduction of PVMs on the composite system 'AE' to the system 'A'. Again, we have to be careful about the initial state since entanglement might prevent us from obtaining a well-defined reduced description. Consider the situation, where the composite system 'AE' is in a product quantum state $\rho_A \otimes \sigma_E \in D(\mathcal{H}_A \otimes \mathcal{H}_E)$ for a fixed quantum state $\sigma_E \in D(\mathcal{H}_E)$ (not neccessarily pure). Measuring this product state with the PVM $\{P_n^{AE}\}_{n\in\mathbb{N}} \subset \text{Proj}(\mathcal{H}_A \otimes \mathcal{H}_E)$ results in measurement outcome $n \in \{1, \ldots, N\}$ with probability

$$p_n = \text{Tr}\left[(\rho_A \otimes \sigma_E) P_n^{AE}\right] = \text{Tr}\left[\rho_A Q_n^A\right], \tag{8}$$

for the operators

$$Q_n^A = \text{Tr}_E\left[(\mathbb{1}_{\mathcal{H}_A} \otimes \sigma_E) P_n^{AE}\right].$$

It can be checked that $Q_n^A \in B(\mathcal{H}_A)^+$ for every $n \in \{1, \ldots, N\}$ and $\sum_{n=1}^N Q_n^A = \mathbb{1}_{\mathcal{H}_A}$. These properties guarantee that the numbers p_n are positive and add up to 1, i.e., that they define a probability distribution. The set of positive operators $\{Q_n^A\}_{n=1}^N$ satisfying $\sum_{n=1}^N Q_n^A = \mathbb{1}_{\mathcal{H}_A}$ is a special instance of a *positive operator-valued measure (POVM)*, which are the most general measurements in quantum theory. The general definition is as follows:

Definition 6.1 (POVM)**.** *A set of operators $\{Q_n\}_{n=1}^N \subset B(\mathcal{H})^+$ is called a positive operator-valued measure (POVM) if $\sum_{n=1}^N Q_n = \mathbb{1}_{\mathcal{H}}$.*

Note that this definition is necessary for the numbers defined in (8) to be probabilities for any quantum state ρ_A.

Non-destructive measurements: In the previous section, we have only specified the probabilities of obtaining a given measurement outcome, but not the quantum state of the system after the measurement. Indeed, specifying the POVM $\{Q_n\}_{n=1}^N$ is in general not sufficient to determine the post-measurement state of the system, and it is convenient to regard such a measurement as *destructive*, i.e., the quantum system is considered to be destroyed in the measurement process. What additional information is needed to determine the post-measurement states of the measurement process outlined above? Again, consider a quantum state $\sigma_E \in D(\mathcal{H}_E)$ and a PVM $\{P_n^{AE}\}_{n\in\mathbb{N}} \subset \text{Proj}(\mathcal{H}_A \otimes \mathcal{H}_E)$. Then, measuring the product state $\rho_A \otimes \sigma_E \in D(\mathcal{H}_A \otimes \mathcal{H}_E)$ leads gives the outcome n with the probability in (8). After obtaining the outcome n the reduced density operator on the system 'A' will be

$$\tau_A^{(n)} = \frac{\text{Tr}_E\left[P_n^{AE}(\rho_A \otimes \sigma_E) P_n^{AE}\right]}{\text{Tr}\left[(\rho_A \otimes \sigma_E) P_n^{AE}\right]} = \frac{\sum_{i=1,j=1}^{d_E} K_{n,i,j}\rho_A K_{n,i,j}^\dagger}{\text{Tr}\left[(\rho_A \otimes \sigma_E) P_n^{AE}\right]} = \frac{T_n(\rho_A)}{\text{Tr}\left[T_n(\rho_A)\right]}, \tag{9}$$

for the operators $K_{n,i,j} \in B(\mathcal{H}_A)$ given by

$$K_{n,i,j} = \sqrt{a_i}\,(\mathbb{1}_{\mathcal{H}_A} \otimes \langle j_E|)\, P_n^{AE}\,(\mathbb{1}_{\mathcal{H}_A} \otimes |\phi_i\rangle),$$

where $\sigma_E = \sum_{i=1}^{d_E} a_i |\phi_i\rangle\langle\phi_i|$ is the spectral decomposition of the positive operator σ_E. It is easy to check that the linear maps $T_n : B(\mathcal{H}_A) \to B(\mathcal{H}_A)$ given by

$$T_n(X) = \sum_{i,j=1}^{d_E} K_{n,i,j} X K_{n,i,j}^\dagger ,$$

are completely positive, which implies that each $\tau_A^{(n)}$ is a quantum state, i.e., it is positive and has unit trace. Furthermore, note that

$$\sum_{i,j=1}^{d_E} K_{n,i,j}^\dagger K_{n,i,j} = \mathrm{Tr}_E \left[\left(\mathbb{1}_{\mathcal{H}_A} \otimes \sigma_E \right) P_n^{AE} \right] = Q_n^A ,$$

which are the operators of the POVM considered in the previous paragraph. This implies

$$\mathrm{Tr}\left[\sum_{n=1}^{N} T_n(X) \right] = \mathrm{Tr}[X] , \tag{10}$$

such that the statistical mixture of post-measurement states

$$\sum_{n=1}^{N} p_n \tau_A^{(n)} = \sum_{n=1}^{N} \mathrm{Tr}\left[T_n(\rho_A) \right] \tau_A^{(n)} = \sum_{n=1}^{N} T_n(\rho_A) ,$$

is a quantum state as well. The set $\{T_n\}_{n=1}^N$ represented by operators $K_{n,i,j}$ as above and satisfying (10) is a special instance of an *instrument*, which are the most general non-destructive measurements in quantum theory. The formal definition is as follows:

Definition 6.2 (Instruments)**.** *A set $\{T_n\}_{n=1}^N$ of completely positive maps $T_n : B(\mathcal{H}_A) \to \mathcal{H}_B$ is called an* instrument *if the sum $T = \sum_{n=1}^N T_n$ is a quantum channel.*

7 The formalism of quantum theory

We can now combine all the insights from the previous section to state the postulates of quantum theory in their modern form. The first postulate stays the same as before, and we merge it with the postulate for composing quantum systems:

Postulate 1 (State space)**.**

1. *For every quantum system, there is an associated complex Euclidean space $\mathcal{H}$ called the* state space*.*
2. *The state space of a composite quantum systems 'AB' arises as the tensor product $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ from the state spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ of its subsystems.*

The second postulate is modified using the notion of density operators introduced above:

Postulate 2 (Quantum states)**.** *The states of a quantum system with state space $\mathcal{H}$ are represented by density operators $\rho \in D(\mathcal{H})$, which we simply call* quantum states*.*

As before, we will say that a quantum state $\rho \in D(\mathcal{H})$ is pure, if it coincides with a rank-1 projection, i.e., if $\rho = |\psi\rangle\langle\psi|$ for some unit vector $|\psi\rangle \in \mathcal{H}$. Note that the pure states are the extreme points of the convex set $\rho \in D(\mathcal{H})$.

The next definition is slightly more general than what we have discussed above. When considering general physical transformations, i.e., all transformations that can be obtained by combining partial traces and time-evolutions, there is no reason that the dimension of the input system and the output system should coincide. However, it is easy to see by the same reasoning as above that such maps still need to be completely positive and trace-preserving. This justifies the following:

Postulate 3 (Quantum channels)**.** *The physical transformations of a quantum system 'A' into a quantum system 'B' is represented by a quantum channel* $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$*, i.e., a trace-preserving and completely positive map.*

A special case of a quantum channel is a *unitary quantum channel* $T : B(\mathcal{H}) \to B(\mathcal{H})$ given by $T(X) = UXU^\dagger$ for a unitary $U \in \mathcal{U}(\mathcal{H})$. Therefore, the notion of quantum channel contains the time-evolutions of closed systems as a special case. Quantum channels are, in general, not reversible, i.e., their inverse is usually not a quantum channel[3]. Examples of irreversible quantum channels are, e.g., the *constant quantum channels* $T : B(\mathcal{H}_A) \to B(\mathcal{H}_B)$ given by $T(X) = \mathrm{Tr}[X]\,\sigma$ for some fixed quantum state $\sigma \in D(\mathcal{H}_B)$.

When discussing measurements, we have the two notions of destructive and non-destructive measurements:

Postulate 4 (Measurements and instruments)**.** *When measuring a quantum system we distinguish the following cases:*

- ***Destructive measurements:*** *They are modelled by a POVM* $\{Q_n\}_{n=1}^N$*, i.e., a set of positive operators satisfying* $\sum_{n=1}^N Q_n = 1$*. Measuring a quantum state* $\rho \in D(\mathcal{H})$ *results in the measurement outcome* n *with probability*

$$p_n = \mathrm{Tr}\left[\rho Q_n\right].$$

- ***Non-destructive measurements:*** *They are modelled by an instrument* $\{T_n\}_{n=1}^N$*, i.e., a set of completely positive maps such that* $\sum_{n=1}^N T_n$ *is a quantum channel. Measuring a quantum state* $\rho \in D(\mathcal{H})$ *results in the measurement outcome* n *with probability*

$$p_n = \mathrm{Tr}\left[T_n(\rho)\right],$$

and after obtaining outcome n *the quantum state of the system is*

$$\rho_n = \frac{T_n(\rho)}{\mathrm{Tr}\left[T_n(\rho)\right]}.$$

Some authors would not use the terms non-destructive measurements and instruments as synonyms, but to us this seems like a rather arbitrary distinction and we will keep the terminology introduced here. We will also continue to use the term PVM to mean a POVM in which all operators are orthogonal projections.

Now, we have formulated the postulates of quantum theory. By our discussion from the previous sections, these postulates contain all states, time-evolutions and measurements of open quantum systems. Since our new postulates contain the old postulates for closed quantum systems as special cases (pure quantum states are the states of closed systems, unitary quantum channels describe their time-evolution, etc.) it is clear that they are more general. In the next section we will see that the two sets of postulates are in fact equivalent. Given any object in the theory of open quantum systems it is always possible to dilate it to an object in the theory of closed quantum systems.

[3] It can be shown that a quantum channel $T : B(\mathcal{H}) \to B(\mathcal{H})$ is reversible if and only if it is a unitary quantum channel.