Chapter 5

Open system dynamics

Idea

We discuss in this chapter basic tools for the time evolution of an "open quantum system" – where the Schrödinger equation alone is not sufficient because the system exchanges energy and information with its environment. In the context of (quantum) information processing, the formalism can be applied to a channel that transmits information: one inputs an initial state and gets out a final one, generally a different one due to noise that has crept in.

Starting from a few physically well-motivated assumptions, we shall derive a surprisingly precise characterization of the possible dynamics. The time evolution of an open quantum system can be understood as a mapping $\hat{\rho}(0) \mapsto \hat{\rho}(t)$ between density matrices. This mapping must satisfy some constraints, for example, it must preserve the probability interpretation of quantum mechanics. In addition, it seems reasonable that initial density matrixes that are "mixtures" of pure states evolve in a linear way and remain mixtures.

5.1 Mixed states

(lecture 03 Dec 14) Motivations:
– generalize state vectors $|\psi\rangle \in \mathcal{H}$ in Hilbert space (remove reduncancy of un-observable global phase)

– combine classical probability (ignorance) about preparation with quantum expectation values
– describe measurements on a 'part of a bigger system'. This is typical for quantum communication protocols.

5.1.1 Definition

A *density operator* is a hermitean operator ρ on the Hilbert space $\mathcal{H}$ of the quantum system under consideration, with the properties

- ρ is positive, i.e., $\langle\psi|\rho|\psi\rangle \geq 0$ for all $\psi \in \mathcal{H}$
- ρ is a trace class operator, i.e., the trace $\mathrm{tr}\,\rho = \sum_n \langle n|\rho|n\rangle < \infty$ exists. Here the vectors $|n\rangle$ form a basis of $\mathcal{H}$. Often one requires ρ to be normalized in trace so that $\mathrm{tr}\,\rho = 1$.

It is easy to see the inequality $0 \leq \langle\psi|\rho|\psi\rangle \leq 1$ for a normalized state vector. Physically, this means that this real number can be interpreted as a probability: it is the probability to find the system in the state $|\psi\rangle$ when performing a measurement.

The expectation value of an operator A is now given by the rule

$$\langle A\rangle_\rho = \mathrm{tr}\,(A\rho) = \mathrm{tr}\,(\rho A) \tag{5.1}$$

where the order under the trace can be changed because of cyclic permutations.

Exercise. Show that for a normalized state $|\psi\rangle \in \mathcal{H}$, the projector

$$\rho = |\psi\rangle\langle\psi| \tag{5.2}$$

is a density operator. Density operators of this form are called 'pure states'.

Exercise. Show that for two density operators ρ_1, ρ_2, the 'mixture' (also known as 'convex sum')

$$\rho = p\rho_1 + (1-p)\rho_2\,, \qquad 0 \leq p \leq 1 \tag{5.3}$$

is also a density operator.

5.1.2 Examples

Preparation with incomplete information

A machine that produces states $|\psi_n\rangle$ with probabilities p_n. Define expectation values by combining quantum and classical averages. For operator A:

$$\langle A\rangle = \sum_n p_n \langle\psi_n|A|\psi_n\rangle \tag{5.4}$$

where the matrix element $\langle\psi_n|A|\psi_n\rangle$ gives the 'quantum average' and the summation over n the 'classical average'.

Exercise. This formula can be re-written in the form

$$\langle A\rangle = \sum_n p_n \,\mathrm{tr}\,(A|\psi_n\rangle\langle\psi_n|) = \mathrm{tr}\,(A\rho) \tag{5.5}$$

where the density operator that appears here

$$\rho = \sum_n p_n \,|\psi_n\rangle\langle\psi_n| \tag{5.6}$$

is also called a 'mixture'. Note that this procedure does not require that the states $|\psi_n\rangle$ are orthogonal or complete.

Partial measurement: reduced density operator

Tensor product structure of a 'bigger system' with two parts A and B. One can think of particles that are available to 'Alice' and 'Bob' in spatially separate locations. But other cases also appear, like large and small scales.

Tensor product of basis states

$$|n,m\rangle = |n\rangle \otimes |m\rangle\,, \tag{5.7}$$

of Hilbert spaces

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B\,, \tag{5.8}$$

of operators

$$A|n,m\rangle = (A\otimes \mathbb{1})|n\rangle\otimes|m\rangle = (A|n\rangle)\otimes|m\rangle\,, \tag{5.9}$$

and the rule for scalar products and matrix elements

$$\langle n, m|A|n', m'\rangle = \langle n|A|n'\rangle\langle m|m'\rangle = \langle n|A|n'\rangle\delta_{mm'} \tag{5.10}$$

A state like $|n\rangle \otimes |m\rangle$ in Eq.(5.7) is called a 'product state' and it does not contain any 'interesting correlations'. For observables A and B of Alice and Bob, calculate

$$C_{AB} = \langle AB\rangle - \langle A\rangle\langle B\rangle = 0 \tag{5.11}$$

Here, the product should actually be understood as $AB = A \otimes B$. Note and think twice about that the commutator

$$[A \otimes \mathbb{1}, \mathbb{1} \otimes B] = 0 \tag{5.12}$$

for a 'trivial' reason. Hence even if A and B are non-commuting, the fact that they are measured in separate systems makes them simultaneously observable. (This also illustrates why the time difference: 'who measures first?' is irrelevant.)

The *reduced density operator* ρ_A is encoding all possible measurements of 'local observables':

$$\langle A \otimes \mathbb{1}\rangle = \mathrm{tr}\,(A\rho_A) \tag{5.13}$$

If the 'global state' is ρ_{AB} or $|\Psi_{AB}\rangle$, one often uses the notation

$$\rho_A = \mathrm{tr}_B(\rho_{AB}) = \mathrm{tr}_B(|\Psi_{AB}\rangle\langle\Psi_{AB}|) \tag{5.14}$$

and says: 'take the partial trace' or 'trace out Bob's Hilbert space'. The precise definition is given here in terms of the matrix elements of ρ_A:

$$\langle n|\rho_A|n'\rangle = \sum_m \langle n, m|\rho_{AB}|n', m\rangle \tag{5.15}$$

where the word 'partial trace' arises because one is summing over diagonal matrix elements in Bob's 'factor' of the Hilbert space.

Exercise. Check that Eq.(5.15) is consistent with the definition (5.13).

Thermal states

In a sense, thermal quantum states are a natural generalization of classical thermodynamics to the quantum world. One uses stationary states, hence the number states we found first, and imposes Boltzmann statistics to describe the field at thermal equilibrium.

For a system with the Hamiltonian H, the thermal state is given by a density operator that generalizes the Boltzmann factor of classical statistical mechanics:

$$\rho = \frac{1}{Z}\exp(-H/k_BT) = \frac{1}{Z}\sum_n \mathrm{e}^{-E_n/k_BT}|n\rangle\langle n| \tag{5.16}$$

where $|n\rangle$ are the stationary states with energy eigenvalue E_n. The normalization factor Z is found by requiring that the trace of this operator be unity:

$$Z = \mathrm{tr}\,\exp(-H/k_BT) = \sum_n \mathrm{e}^{-E_n/k_BT} \tag{5.17}$$

You know this sum from classical thermodynamics as 'partition function' (*Zustandssumme*). The normalized probabilities

$$p_n(T) = \frac{\mathrm{e}^{-E_n/k_BT}}{Z} \tag{5.18}$$

are simply the classical probability that the stationary state $|n\rangle$ is realized in the canonical ensemble.

We note that the terms $|n\rangle\langle n|$ in the sum (5.16) are also density operators: they are obviously positive and have trace unity. (In fact, the trace boils down to the norm squared of the state $|n\rangle$.) The thermal density operator is thus a probability-weighted, convex sum of density operators.[1] This convex summation is, in general, an allowed linear operation on the space of density operators.

Pure states and purity

The density operators $|n\rangle\langle n|$ are special because they are made up of a single state. These quantum states are called *pure*. A formal definition:

[1] One talks about a *convex sum* if all coefficients are real numbers between zero and one.

- A density operator ρ describes a *pure state* if $\rho^2 = \rho$.

In mathematics, operators with this property are called *projectors*. This is also what is suggested by the Dirac notation $|\psi\rangle\langle\psi|$: this operator acts on the Hilbert space by first projecting onto the state $|\psi\rangle$ and then gives back a vector proportional to $|\psi\rangle$, just what happens in geometry for the projection onto a vector.

States that are not pure are called 'mixed'. This can be made more quantitative:

- The *purity* of a density operator ρ is defined by

$$\mathrm{Pu}(\rho) = \mathrm{tr}\left(\rho^2 - \rho\right) + 1 = \mathrm{tr}\,\rho^2 \tag{5.19}$$

  where the two definitions are equal if ρ is trace-normalized.

The purity is normalized such that for pure states, $\mathrm{Pu}(\rho) = 1$. It is easy to see that the first term in (5.19), $\mathrm{tr}\,(\rho^2 - \rho)$ is negative for mixed states. One can also show that $\mathrm{Pu}(\rho) = 1$ is equivalent to the state being pure.

To show these properties, evaluate the trace of ρ^2 in the eigenbasis of ρ. All eigenvalues are in the interval $[0, 1]$.

5.2 Dynamical maps

We define a "dynamical map" $T : \rho(0) \mapsto \rho(t) = T[\rho(0)]$ as a linear map of density matrices to density matrices. Actually, we only need "convex linearity" because this is the canonical way to generate mixed states:

$$T(\sum_k p_k \rho_k) = \sum_k T(\rho_k), \qquad p_k \geq 0, \sum_k p_k = 1 \tag{5.20}$$

but this construction is easily generalized to linear combinations with complex coefficients.

We start from the intuitive picture that T implements the time evolution of the density operator to state the following, apparently obvious properties for a "dynamical map" T.

Definition: dynamical map.

the map $T : \rho(0) \mapsto \rho(t) = T[\rho(0)]$ is linear (clearly motivated by convex sums as input states)

domain (*Definitionsbereich*) of the map T: all (initial) density operators $\rho(0)$

the image $\rho(t)$ is a density operator: hermitean, non-negative, and of trace unity. One calls the map itself therefore trace-preserving and "positive".

the map T is completely positive, as explained now.

"Complete positivity" means the following: imagine that we enlarge the space on which ρ operates and extend T in the following way to "larger" density matrices P. For factorized matrices, $\mathrm{P} = \rho \otimes \rho_{\mathrm{B}}$, we set

$$(T \otimes \mathbb{1})(\mathrm{P}) = T(\rho) \otimes \rho_{\mathrm{B}} \tag{5.21}$$

and extend this to arbitrary ("entangled") operators P by linearity. We then require that the extended map $(T \otimes \mathbb{1})$ is positive for any dimension of the extended space.

There are physical time evolutions that do not fit into this framework. For example, it is possible that the initial density operator $\hat{\rho}(0)$ for an open system does not contain enough information about the system–environment correlations to predict the system's future. See Pechukas (1994).

At first sight, complete positivity looks as a quite natural condition, not a very strong constraint. It reveals its full power as soon as non-factorized states P on the larger Hilbert space ("entangled states") enter the game.

5.3 Characterization of completely positive maps

It may come as a surprising fact that these conditions already imply a very special form for the dynamical maps: this is the

Kraus-Stinespring representation theorem: All dynamical maps are of the form

$$T(\rho) = \sum_k \Omega_k \rho \Omega_k^\dagger \tag{5.22}$$

with $\sum_k \hat{\Omega}_k^\dagger \hat{\Omega}_k = \mathbb{1}$.

Note that this equation generalizes the unitary evolution that we recover when the sum over the "Kraus operators" Ω_k contains only a single term. Exercise: Eq.(5.22) defines a completely positive map and preserves the trace of ρ.

Sketch of a proof. Adapted from Chap. 4 in *Quantum Computing Devices: Principles, Designs and Analysis* by G. Chen & al, Taylor & Francis 2006, itself taken from Nielsen & Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press 2000).

You prove in the exercises that Eq.(5.22) defines a completely positive map. The only tricky point is the following extension to density operators P in a larger space

$$(T \otimes \mathbb{1})(P) = \sum_k (\Omega_k \otimes \mathbb{1}) P (\Omega_k^\dagger \otimes \mathbb{1}) \tag{5.23}$$

where the factor $\otimes\mathbb{1}$ provides the necessary extension to larger dimensions.

We now want to prove the converse. Consider the extended Hilbert space $\mathcal{H} \otimes \mathcal{H}$. Take a vector $|\phi\rangle \in \mathcal{H} \otimes \mathcal{H}$ and construct the operator

$$P = (T \otimes \mathbb{1})(|\phi\rangle\langle\phi|) \tag{5.24}$$

Since T is completely positive, and $|\phi\rangle\langle\phi|$ is a density operator, P is a (positive) density operator. Since P is hermitean, its spectral representation exists and can be written in the form

$$P = \sum_k |\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k|. \tag{5.25}$$

We have lumped the non-negative eigenvalues into the non-normalized eigenvectors $|\tilde{\varphi}_k\rangle$.

We now construct linear maps Ω_k on the system Hilbert space. Let $|\psi\rangle, |\chi\rangle \in \mathcal{H}$. Define the ket $|\psi^\star\rangle$ with respect to a basis $\{|n\rangle\}$ of $\mathcal{H}$ by "taking the complex conjugate of the coefficients", i.e.:

$$|\psi^\star\rangle = \sum_n |n\rangle\langle n|\psi^\star\rangle, \qquad \langle n|\psi^\star\rangle \equiv (\langle n|\psi\rangle)^* = \langle\psi|n\rangle \tag{5.26}$$

The Kraus operators are now defined via their matrix elements as

$$\langle\chi|\Omega_k|\psi\rangle = \langle\chi\otimes\psi^\star|\tilde{\varphi}_k\rangle, \qquad \langle\psi|\Omega_k^\dagger|\chi\rangle = \langle\tilde{\varphi}_k|\chi\otimes\psi^\star\rangle, \tag{5.27}$$

where the adjoint operator is defined in the usual way. We use the notation $\langle\chi\otimes\psi^\star|$ for the tensor product between the bras (linear forms) $\langle\chi|$ and $\langle\psi^\star|$.

Let us now analyze the following matrix elements of the image density operator P, taking arbitary $|\chi\rangle, |\chi'\rangle, |\psi\rangle \in \mathcal{H}$

$$\begin{aligned}
&\langle\chi\otimes\psi^\star|P|\chi'\otimes\psi^\star\rangle \\
&= \sum_k \langle\chi\otimes\psi^\star|\tilde{\varphi}_k\rangle\langle\tilde{\varphi}_k|\chi'\otimes\psi^\star\rangle \qquad \text{from Eq.(5.25)} \\
&= \sum_k \langle\chi|\Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger|\chi'\rangle
\end{aligned} \tag{5.28}$$

We now specialize to the following form for the vector $|\phi\rangle \in \mathcal{H}\otimes\mathcal{H}$:

$$|\phi\rangle = \sum_n |n\otimes n\rangle \tag{5.29}$$

(this vector is a so-called maximally entangled state on the product Hilbert space). Its projector admits the following expansion

$$\begin{aligned}
|\phi\rangle\langle\phi| &= \sum_{n,m} |n\otimes n\rangle\langle m\otimes m| \\
&= \sum_{n,m} (|n\rangle\langle m|)\otimes(|n\rangle\langle m|)
\end{aligned} \tag{5.30}$$

in terms of skew operators $|n\rangle\langle m|$. It is quite astonishing that the full knowledge about T can be obtained by applying its extension (Eq.(5.24) to this single projector. We shall see in a moment that a dynamical map T (and its extensions) can be defined on skew operators as well, Eq.(5.35). Taking this for granted, we get

$$P = (T\otimes\mathbb{1})(|\phi\rangle\langle\phi|) = \sum_{n,m} T(|n\rangle\langle m|)\otimes(|n\rangle\langle m|) \tag{5.31}$$

Using the definition (5.26), we find that the matrix element of Eq.(5.28) becomes

$$\begin{aligned}
&\sum_{n,m} (\langle\chi|\otimes\langle\psi^\star|)\,[T(|n\rangle\langle m|)\otimes(|n\rangle\langle m|)]\,(|\chi'\otimes\psi^\star\rangle) \\
&= \sum_{n,m} \langle\chi|T(|n\rangle\langle m|)|\chi'\rangle\langle n|\psi\rangle\langle m|\psi\rangle^* \\
&= \langle\chi|T(|\psi\rangle\langle\psi|)|\chi'\rangle.
\end{aligned} \tag{5.32}$$

In the last step, we have used the expansion of $|\psi\rangle$ in the basis $\{|n\rangle\}$.

Combining with Eq.(5.28), we have shown that

$$\langle\chi|T(|\psi\rangle\langle\psi|)|\chi'\rangle = \sum_k \langle\chi|\Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger|\chi'\rangle \tag{5.33}$$

Now, the vectors $|\chi\rangle$, $|\chi'\rangle$ are arbitary and hence

$$T(|\psi\rangle\langle\psi|) = \sum_k \Omega_k|\psi\rangle\langle\psi|\Omega_k^\dagger \tag{5.34}$$

Hence, we have proven the operator identity (5.22) for the special case of a pure state $\rho = |\psi\rangle\langle\psi|$. The proof is extended to a mixed state by decomposing ρ into projectors $|\psi_i\rangle\langle\psi_i|$ onto eigenvectors with non-negative weights (eigenvalues) p_i, and using the linearity of T.

To fill the gap, we need a prescription to apply a dynamical map to skew operators. We assume that $|\psi\rangle$ and $\chi\rangle$ are orthogonal and set

$$\begin{aligned} T(|\psi\rangle\langle\chi|) &= \frac{1}{2}\left[T(\rho_{+1}) - T(\rho_{-1}) + iT(\rho_{+i}) - iT(\rho_{-i})\right] \\ \rho_u &:= \frac{1}{2}\left[(|\psi\rangle + u|\chi\rangle)(\langle\psi| + u^*\langle\chi|)\right], \qquad |u| = 1 \end{aligned} \tag{5.35}$$

where T is applied to projectors onto superposition states of ψ and χ with suitably chosen phase factors u. For a complex linear map, Eq.(5.35) is actually trivially satisfied, as a direct calculation shows. (See exercises.)

Last gaps to fill. Check that the Kraus operators resolve the identity, $\sum_k \Omega_k^\dagger\Omega_k = \mathbb{1}$.

Remarks

- A map is completely positive if it is positive on the "doubled Hilbert space". This is actually all that we needed in the proof.
- If D is the dimension of the Hilbert space $\mathcal{H}$, then there are at most D^2 Kraus operators Ω_k. This is the maximum number of eigenvectors of P with nonzero eigenvalue (the maximum rank of P).
- The vector space of all linear maps is (at most) of dimension D^4: these "superoperators" can be written as $D^2 \times D^2$ matrices that act

on the D^2-dimensional space of density matrices. (All dimensional estimates are actually upper limits here.) This suggests that the completely positive maps only cover a small subspace of all linear maps, in particular if D is large.

- The Kraus theorem provides us a characterization of all completely positive maps. Current research is turned towards a similar result for "positive maps". These maps, extended to the double Hilbert space, may image density operators onto operators with negative eigenvalues. This is connected to the generation of entanglement between the system and its "copy".

- There are researchers who do not accept the requirement of complete positivity (Pechukas, *Phys Rev Lett* 1994): they maintain that factorized states actually never occur in Nature (there are always some correlations or entanglement with the "rest of the world"). From this viewpoint, the violation of complete positivity is related to the fact that the (forgotten) correlations between the system and its environment are needed to construct the proper time evolution. In this sense, time evolution need not be a (completely) positive map. A pragmatic solution ('Who's afraid of not completely positive maps?', Shaji and Sudarshan, *Phys Lett A* 2005) could be to restrict the application of a given (approximate) dynamical map to a subset of initial density operators where the map is completely positive.

- Current research is aimed at extending or exploiting the Kraus theorem to master equations "with memory" (non-Markov case). At the time of writing, there are a few generalizations attempted, but no general result has been proven.

5.3.1 Remarks and examples

Choi matrix. The density operator P defined in Eq.(5.31) is called the Choi matrix of the map T. The following re-formulation of the Kraus-Stinespring theorem is called the **Choi theorem**: the map T is completely positive if and only if its Choi matrix P is positive.

Random unitary. Imagine that you have a Hamiltonian $H(x)$ that depends on a "random parameter" x. It can take the values $x = x_k$ with probability p_k. This happens, for example, in your laboratory class when certain values of your apparatus are not well controlled. Then we can define the following "average density matrix" (denoted by the overbar) after time evolution under the unitary operator $U(x) = \exp[-\mathrm{i}H(x)t]$:

$$\rho \mapsto \overline{U(x)\rho U^\dagger(x)} = \sum_k p_k U(x_k)\rho U^\dagger(x_k) \tag{5.36}$$

Actually, from a quantum-mechanical perspective, this is the only way to describe the "preparation procedure" that you implement with the non-accurately known Hamiltonian. We observe that Eq.(5.36) is of the form of the Kraus theorem, with $\Omega_k = \sqrt{p_k}U(x_k)$.

Stinespring dilation theorem. Formulation for a physicist: every completely positive map can be represented by a unitary map on a larger Hilbert space, followed by a partial trace. The projection procedure in the 'system+bath' approach is therefore also the only way to construct a completely positive map.

The main idea is to collect the Kraus operators Ω_k ($k = 1 \ldots K$) into a block-diagonal matrix

$$U = \begin{pmatrix} \Omega_1 & & & \\ & \Omega_2 & & \\ & & \ddots & \\ & & & \Omega_n \end{pmatrix} \tag{5.37}$$

where the basis $\{|n,k\rangle\}$ is chosen with an 'ancilla' system $\mathcal{K}$ of dimension K. It is easy to check that this gives a unitary matrix U on the enlarged Hilbert space and the representation

$$T(\rho) = \mathrm{tr}_{\mathcal{K}}[U(\rho \otimes K^{-1}\mathbb{1})U^\dagger] \tag{5.38}$$

where $K^{-1}\mathbb{1}$ is a completely mixed state on $\mathcal{K}$. The Kraus operators of the completely positive map thus encode a 'reversible' evolution if the quantum system ('ancilla') keeps track of which Kraus operator Ω_k has been applied. As long as the ancilla is not measured (no partial trace taken), the state remains pure on the enlarged Hilbert space.

GNS purification (after Gelfand and Naimark, and Segal). Generalize CP maps between different Hilbert spaces (i.e., the set of density operators). Read a state ρ as such a generalized CP map. The Stinespring dilation theorem allows to represent this as a pure state

$$\rho = \mathrm{tr}_2|\Psi\rangle\langle\Psi| \qquad |\Psi\rangle = \sum_n \sqrt{p_n}|n \otimes n\rangle, \qquad \rho = \sum_n p_n|n\rangle\langle n| \tag{5.39}$$

where the states $|n\rangle$ are the eigenvectors of ρ with eigenvalues p_n. The pure state $|\Psi\rangle$ is a superposition of eigenvectors tensorized with themselves: as long as the 'ancilla system' keeps a copy of the eigenvector, purity is not lost.

5.3.2 Nakajima–Zwanziger map

System+bath projector. The names Nakajima and Zwanziger are attached to the following natural prescription for the reduced density operator of a system coupled to a bath. This map a actually a completely positive map. We pick a fixed state ρ_B for the bath; this state is an equilibrium state of the bath, and specifies the bath parameter "temperature". Construct from this and the system density operator $\rho(0)$ an initial system+bath state as a tensor product $P(0) = \rho(0) \otimes \rho_B$ (this is a capital ρ). Then evolve this state with a Hamiltonian H_{SB} that contains everything: system and bath Hamiltonian and their mutual coupling. In terms of the corresponding unitary time evolution

$$P(0) \mapsto P(t) = U_{SB}(t)P(0)U_{SB}^\dagger(t) \tag{5.40}$$

Finally, at time t, the system density operator is obtained in the usual way as a reduced density operator (tracing out the bath degrees of freedom), $\rho(t) = \mathrm{tr}_B[P(t)]$. Putting everything together we have the Nakajima-Zwanziger formula

$$\rho(0) \mapsto \rho(t) = \mathrm{tr}_B\left[U_{SB}(t)\rho(0) \otimes \rho_B U_{SB}^\dagger(t)\right] \tag{5.41}$$

Exercise: show that this defines a completely positive map.

5.3.3 Partial transpose

Definition. For an operator ρ on a bipartite Hilbert space, consider a tensor product basis $\{|n,m\rangle\}$ and define the partially transposed operator ρ^Γ (the superscript is half a letter T) by its matrix elements

$$\langle n,m|\rho^\Gamma|n',m'\rangle = \langle n,m'|\rho|n',m\rangle \tag{5.42}$$

(No complex conjugation here; partially transpose does not mean "partially hermitean conjugate".)

The partial transpose is a linear map, but it does not preserve positivity. To see this, consider a two-qubit Hilbert space and the pure state

$$\rho = |\psi_+\rangle\langle\psi_+| \quad \text{with} \quad |\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \tag{5.43}$$

In the basis $\{|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle\}$, this projector and its partial transpose are represented by the matrix (please check it)

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \qquad \rho^\Gamma = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{5.44}$$

The determinant of ρ^Γ is -1, hence one eigenvalue must be negative, and ρ^Γ is not positive.

Note from Eq.(5.42) that the partial transpose is the natural extension of the transposition T to an enlarged Hilbert space: $\Gamma = \mathbb{1}\otimes\mathrm{T}$. We therefore conclude that the transposition is not a completely positive map.

The transposition is closely related to the complex conjugation of each matrix element of a density matrix, $\rho_{mn} \mapsto \rho^*_{mn}$: this is easy to see since ρ is hermitean and therefore invariant under hermitean conjugation = transpose and conjugate. It is interesting to realize that the "simple" conjugation is often related to time reversal. The statement above thus suggests the following conjecture: if we time-reverse the evolution of a subsystem, letting the "rest" evolve forward in time as usual, then this dynamics may lead to negative probabilities.

5.4 The Lindblad master equation

The Lindblad (Gorini-Kossakowski-Sudarshan) theorem provides an equation of motion for the density operator in terms of a differential equation.

In technical terms, the time evolution is supposed to be given by a family of completely positive (dynamical) maps that form a semigroup. The Lindblad theorem gives the (time-independent) generator of this semigroup. This result is sometimes called a Markovian master equation because it gives the time evolution of the density operator at time t in terms of $\rho(t)$ (the past is not important).

Semigroup. A family of dynamical maps $\{T_t | t \geq 0\}$ that can be concatenated (*hintereinander ausführen*). Indeed, it is plausible that the time evolutions $\rho(0) \mapsto \rho(t) = T_t(\rho(0))$ can be applied repeatedly,

$$T_{t_1+t_2} = T_{t_1} T_{t_2} \tag{5.45}$$

and the result is also a time evolution. What is missing from the usual group property: inverse element "T_{-t}". Evolution is always "forward in time only" (related to dissipation and loss of information).

Eq.(5.45) is a "functional equation" that is formally solved by an operator of exponential form

$$T_t = \exp(\mathcal{L}t) \tag{5.46}$$

where $\mathcal{L}$ is called the "generator" of the semigroup; it is itself time-independent. (The exponential map provides the homomorphism between concatenation of dynamical maps and addition of the time arguments.) Similar to the Kraus theorem, the constraints of linearity and complete positivity specify the structure of the generator. This is the so-called

5.4.1 Lindblad theorem

A completely positive semigroup $T_t = \exp(\mathcal{L}t)$ has a generator $\mathcal{L}$ that implements the time evolution of a density operator ρ in the form of the following differential equation. There is a hermitean operator H and a countable family of operators L_k (acting on the Hilbert space of the system) with

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\mathrm{i}\,[H,\,\rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \left\{ \rho, L_k^\dagger L_k \right\} \right) \\ &= -\mathrm{i}\,[H,\,\rho] + \frac{1}{2} \sum_k \left(\left[L_k \rho,\, L_k^\dagger \right] + \left[L_k,\, \rho L_k^\dagger \right] \right) \end{aligned} \tag{5.47}$$

The following sketch of a proof is adapted from Nielsen & Chuang and C. Henkel, *J Phys B* 2007. A slightly different version can be found in the book by Breuer & Petruccione (2002).

We evaluate the difference quotient

$$\frac{\rho(t+\Delta t)-\rho(t)}{\Delta t} \tag{5.48}$$

with the help of the Kraus theorem and take the limit $\Delta t \to 0$. Write $\rho = \rho(t)$ for simplicity. In the Kraus representation (5.22) for the density matrix $\rho(t+\Delta t)$,

$$\rho(t+\Delta t) = \sum_k \Omega_k \rho \Omega_k^\dagger \tag{5.49}$$

the operators Ω_k depend on Δt. They can be split into

$$\Omega_k = \omega_k \mathbb{1} + V_k \tag{5.50}$$

where the first term contains the term proportional to the unit operator. This splitting can be made unique using the following scalar product on the space of operators:

$$(A|B) = \mathrm{tr}(A^\dagger B) \tag{5.51}$$

Hence, the projection of Ω_k orthogonal to $\mathbb{1}$ which is V_k must satisfy

$$0 = (\mathbb{1}|V_k) = \mathrm{tr}(\mathbb{1}V_k) = \mathrm{tr}\, V_k \tag{5.52}$$

in other words, it is traceless. Note that both ω_k and V_k depend on Δt.

In terms of these quantities, the change in the density matrix is computed to be

$$\begin{aligned} &\rho(t+\Delta t) - \rho \\ &= (\sum_k |\omega_k|^2 - 1)\rho + \sum_k \left(\omega_k^* V_k\, \rho + \rho\, \omega_k V_k^\dagger\right) + \sum_k V_k^\dagger \rho V_k \end{aligned} \tag{5.53}$$

where ω_k^* is complex conjugate to ω_k. We assume that the following continuity condition holds

$$\lim_{\Delta t \to 0} \left[\hat{A}\rho(t+\Delta t) - \hat{A}\rho(t)\right] = \mathcal{O}(\Delta t) \tag{5.54}$$

for all operators $\hat{A}$ and initial density matrices $\rho(t)$. This permits us to extract all matrix elements in Eq.(5.53) and to conclude that the following terms must vanish separately

$$\lim_{\Delta t\to 0}\sum_k |\omega_k|^2 = 1 \tag{5.55}$$

$$\lim_{\Delta t\to 0}\sum_k \omega_k^* \rho V_k \; = 0 \tag{5.56}$$

$$\lim_{\Delta t\to 0}\sum_k V_k\, \rho V_k^\dagger = 0 \tag{5.57}$$

where the last two lines apply to any density matrix ρ. We now assume that the following derivatives exist

$$\gamma \;\equiv\; \lim_{\Delta t\to 0}\frac{\sum_k |\omega_k|^2 - 1}{\Delta t} \tag{5.58}$$

$$\Gamma - iH \;\equiv\; \lim_{\Delta t\to 0}\frac{\sum_k \omega_k^* V_k}{\Delta t} \tag{5.59}$$

where Γ and H are both hermitean.

Differentiating the condition that the dynamical map preserves the trace of the density matrix, we find

$$\begin{aligned} 0 \;&=\; \lim_{\Delta t\to 0}\frac{\mathrm{tr}\,[\rho(t+\Delta t)-\rho]}{\Delta t} \\ &=\; \mathrm{tr}\Big[\gamma\rho + 2\Gamma\rho + \lim_{\Delta t\to 0}\frac{1}{\Delta t}\sum_k V_k^\dagger V_k\,\rho\Big] \end{aligned} \tag{5.60}$$

Since this must hold for any density matrix ρ, we find another derivative (this argument uses that the scalar product (5.51) is non-degenerate)

$$\lim_{\Delta t\to 0}\frac{\sum_k V_k^\dagger V_k}{\Delta t} = -\gamma - 2\Gamma \tag{5.61}$$

We can thus introduce the Lindblad operators L_k by the limiting procedure

$$L_k \equiv \lim_{\Delta t\to 0}\frac{V_k}{\sqrt{\Delta t}} \tag{5.62}$$

where we used that the root of $\Delta t \geq 0$ can be taken. Using the derivatives defined in Eqs.(5.58, 5.59, 5.62), we can divide the difference $\rho(t+\Delta t)-\rho(t)$ in Eq.(5.53) by Δt, and take the limit $\Delta t \to 0$. This gives the differential equation (5.47).

Note that a Lindblad operator L proportional to the unit operator automatically gives a zero contribution in the Lindblad form. This is why the split in Eq.(5.50) makes sense.

5.4.2 Examples

Spontaneous emission

of a two-level atom is described by a single "Lindblad operator"

$$L = \sqrt{\gamma}\,\sigma \tag{5.63}$$

where the strange unit arises because the "square of L" provides the actual time derivative of ρ. This result for spontaneous emission is derived in Sec.**??**.

We can best check that this is compatible with the Born-Markov master equation by switching to the Heisenberg picture. Taking the trace of the Lindblad master equation (5.47), multiplied with a system operator A, we find

$$\frac{\partial}{\partial t}\langle A\rangle = \mathrm{i}\langle[H,\,A]\rangle + \frac{1}{2}\sum_k \left\langle L_k^\dagger\,[A,\,L_k] + \left[L_k^\dagger,\,A\right] L_k\right\rangle \tag{5.64}$$

where the first term is the familiar one. The second one involves commutators between A and the Lindblad operators. Simple calculations show that this leads indeed to the damping of the atomic dipole operators σ and $\sigma^\dagger$ (at the rate γ, Eq.(**??**)) and to the damping of the inversion σ_3, Eq.(**??**), as we found in the previous semester.

Lossy cavity

Let us consider a single-mode cavity with annihilation operator a and consider the non-Schrödinger processes if one mirror is partially transmitting. There are two Lindblad operators that describe the loss of photons from the cavity (bosonic operators a, $a^\dagger$) and the fact that thermal radiation can enter the cavity:

$$L_{\mathrm{loss}} = \sqrt{\kappa(\bar{n}+1)}\,a, \qquad L_{\mathrm{abs}} = \sqrt{\kappa\bar{n}}\,a^\dagger \tag{5.65}$$

where κ is a loss rate (the inverse of the "photon lifetime") and $\bar{n} = (\mathrm{e}^{\hbar\omega_{\mathrm{A}}/k_{\mathrm{B}}T} - 1)^{-1}$ is the average thermal photon number at the cavity frequency. The temperature T corresponds to the radiation field outside the cavity. We recover for $T = 0$ a pure loss channel where the photon annihilation operator in L_{em} plays the role of the atomic ladder operator in Eq.(5.63).

The operator $L_{\rm loss}$ describes the emission of photons (spontaneous and stimulated) into the thermal field; the operator $L_{\rm abs}$ describes photon absorption. This can be easily checked by going back to a two-level model involving only the number states $|0\rangle$ and $|1\rangle$ and working out the equations of motion for the density matrix elements ρ_{00} and ρ_{10}. One gets the rate equations that have been used by Einstein in his proof of the Planck spectrum (*Physikal. Zeitschr.* 1917).

Both rates add up in the dynamics of off-diagonal elements of the density operator ρ_{10} (which plays the role of the atomic dipole, remember the matrix elements $\rho_{\rm eg}$): their decay rate is $\kappa(2\bar{n}+1)$. This is a typical feature of master equations: the off-diagonal elements decay at least with the half-sum of the decay rates of the corresponding populations. In practice, their decay rate is even larger, due to additional dissipative processes ("dephasing").

Dephasing

is a process where only the off-diagonal elements of the density matrix decay, while the populations are left unchanged. The Lindblad operator is

$$L_{\rm deph} = \sqrt{\kappa}\,\sigma_3 \tag{5.66}$$

with a rate κ. By solving the Lindblad master equation (exercise!), we find

$$\rho(t) = \begin{pmatrix} \rho_{\rm ee}(0) & {\rm e}^{-\kappa t}\rho_{\rm eg}(0) \\ {\rm e}^{-\kappa t}\rho_{\rm ge}(0) & \rho_{\rm gg}(0) \end{pmatrix} \tag{5.67}$$

This process can be mimicked in a "classical way" by assuming that a superposition state vector

$$|\psi(t)\rangle = \alpha\,{\rm e}^{{\rm i}\varphi(t)}|{\rm e}\rangle + \beta\,{\rm e}^{-{\rm i}\varphi(t)}|{\rm g}\rangle \tag{5.68}$$

acquires a relative phase $\varphi(t)$ that is "randomly fluctuating". Experimentally, this happens for a two-level system embedded in a solid: the motion of the immediate environment perturbs the form of the electronic orbitals and hence their energy, even if the electron stays in this orbital ("adiabatic perturbation"). Hence only the energy is randomized, but the population is kept constant.

In this context, we can define a quantum-mechanical "average ensemble" by building the density matrix $|\psi(t)\rangle\langle\psi(t)|$ and taking the average over the probability distribution of $\varphi(t)$ (denoted by an overbar):

$$\rho(t) = \overline{|\psi(t)\rangle\langle\psi(t)|} \tag{5.69}$$

With the identification

$$\overline{\mathrm{e}^{\mathrm{i}\varphi(t)}} = \mathrm{e}^{-\kappa t} \tag{5.70}$$

we get the same result as with the Lindblad form. This is true if $\varphi(t)$ is a gaussian random variable with zero average and with variance $\langle\varphi(t)^2\rangle = \kappa t$. This behaviour is similar to Brownian motion (hence the name "phase diffusion"), in the mathematics literature, it is called a "Wiener process".

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