Theory of Open Quantum Systems

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Preface

These notes are intended as a study material for a class on theory of open quantum systems that I thought at ETH Zürich in the spring semester 2014. They do not aim to be a self-contained exposition of the subject. I used several textbooks [8, 12, 5, 2, 16, 14, 1] during the preparation for the class and I often refer to these textbooks instead of rewriting the same material here. The main aim of the lectures was to present the mathematical structure of the theory without using involved language of functional analysis and C^*-algebras. In the range of above mentioned textbooks my exposition is in between mathematically oriented books of Davies [8], Holevo [12], Attal et. al. [2] and more physically minded books of Breuer-Petruccione [5], Alicki-Lendi [1].

1 Introduction

We recall the description of a closed system in quantum mechanics.

Closed system

A state of a closed system S is described (up to a phase) by a normalized vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}_S$. Observables correspond to hermitian operators $A = A^*$, and statistics of measurement outcomes is determined by

$$< A >= \langle\psi|A|\psi\rangle.$$

The evolution of the state is generated by a Hamiltonian H via the Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle.$$

Open system

An open system is made out of two parts, a system S and an environment E:

$$\bar{S} = S \vee E,$$

where $\bar{S}$ is a closed system. The Hilbert space of $\bar{S}$ is a tensor product $\mathcal{H}_S \otimes \mathcal{H}_E$ and states on $\bar{S}$ formed by linear combinations of product states $|\psi\rangle = |\psi_S\rangle \otimes |\psi_E\rangle$. The evolution is generated by a Hamiltonian

$$H = H_S \otimes \mathbb{1} + H_I + \mathbb{1} \otimes H_E,$$

where $H_I = \sum_\alpha A_\alpha \otimes B_\alpha$ describes the interaction between the system and the environment.

The boundary between S and E is arbitrary. The most typical reason to impose the boundary is that only properties of S can (or want to) be measured. However other reasons like separation of scales have to be also considered. The boundary is at the end always just a matter of convenience.

Density matrix and partial trace

Density matrix and partial trace are the most important objects in the theory of open systems. Both were introduced by Landau in his 1927 paper "The damping problem in wave mechanics" and later independently discovered by von Neumann in 1932. We will now follow the exposition of Landau.

Consider a state of the first system described by a wave function ($|\psi_n\rangle$ is a basis)

$$|\psi\rangle = \sum_n a_n |\psi_n\rangle,$$

and a state of the second system

$$|\psi'\rangle = \sum_r b_r |\psi'_r\rangle.$$

The joint wave function for the two systems together is then

$$|\Psi\rangle = |\psi\rangle \otimes |\psi'\rangle = \sum_n \sum_r a_n b_r |\psi_n\rangle \otimes |\psi'_r\rangle = \sum_n \sum_r c_{nr} |\psi_n\rangle \otimes |\psi'_r\rangle,$$

where

$$c_{nr} = a_n b_r.$$

The coefficients c_{nr} depends on time via the Schrödinger equation and if there is a non-trivial coupling between the systems then they can no longer be written in the above dyadic product form.

For an observable $X \otimes \mathbb{1}$ on the first system alone we have

$$< X \otimes \mathbb{1} > = \langle \Psi | X \otimes \mathbb{1} | \Psi \rangle \tag{1}$$

$$= \sum_n \sum_m \sum_r \bar{c}_{nr} c_{mr} \langle \psi_n | X | \psi_m \rangle = \text{tr}(\rho X), \tag{2}$$

where

$$\rho := \sum_m \sum_n \sum_r \bar{c}_{nr} c_{mr} |\psi_m\rangle \langle \psi_n |. \tag{3}$$

Thus the "state" of the system can be described by the quantity ρ. The idea being that a "state" is an information how to prescribe measurement results of a given observable. The quantity ρ is called density matrix. Landau finishes his discussion by pointing out that for the first system alone the corresponding density matrix is

$$\rho = |\psi\rangle \langle \psi|.$$

Basic properties of the density matrix that follow from Eq. (3) are

1. $\rho = \rho^*$;

2. $\text{tr}\,\rho = 1$;

3. $\langle \psi | \rho | \psi \rangle \geq 0$ for all vectors $|\psi\rangle$, such an operator is called positive.

Let us show just the last claim

$$\langle\psi|\rho|\psi\rangle = \sum_m \sum_n \sum_r \bar{c}_{nr}c_{mr}\langle\psi|\psi_m\rangle\langle\psi_n|\psi\rangle = \sum_r \left|\sum_m c_{mr}\langle\psi|\psi_m\rangle\right|^2 \geq 0.$$

From now on we use the word state of a system for a density matrix.

Definition 1 (State) *A state of a system S is a positive operator ρ on $\mathcal{H}_S$, normalized by $\operatorname{tr}\rho = 1$. For a given observable X its expected value is given by*

$$< X > = \operatorname{tr}(\rho X).$$

A pure state corresponding to $|\psi\rangle$ is a projection $P = |\psi\rangle\langle\psi|$.

The equality between (1) and (2) implicitly define the other important object called partial trace. Notice that (1) refers to quantities in the join Hilbert space of the two systems, while (2) refers only to quantities associated to the Hilbert space of the first system.

Definition 2 (Partial trace) *Given a joint state ρ of $S \vee E$ a partial trace $\rho_S = \operatorname{tr}_E(\rho)$ is a unique operator on S for which*

$$\operatorname{tr}_{S\vee E}(\rho X \otimes \mathbb{1}) = \operatorname{tr}_S(\rho_S X).$$

Here $\operatorname{tr}_{S\vee E}$ is the trace in the joint space and tr_S is the trace in the system S alone. The name partial trace is self-explanatory.

A way how to compute the partial trace is following. Write $\rho = \sum_\alpha A_\alpha \otimes B_\alpha$. Then

$$\operatorname{tr}_E(\rho) = \sum_\alpha A_\alpha \operatorname{tr}(B_\alpha).$$

It can be easily checked that this satisfies the definition. Indeed for any observable $X \otimes \mathbb{1}$ we have (we do not anymore write in which space traces are defined it should be clear from their argument)

$$\operatorname{tr}(\rho X \otimes \mathbb{1}) = \operatorname{tr}(\sum_\alpha A_\alpha X \otimes B_\alpha) = \operatorname{tr}(\sum_\alpha A_\alpha X)\operatorname{tr}(B_\alpha)$$
$$= \operatorname{tr}(\operatorname{tr}_E(\rho)X).$$

Remark 3 (Notation) *Partial trace is a map from $B(\mathcal{H}_S) \otimes B(\mathcal{H}_E) \to B(\mathcal{H}_S)$. In fact $\operatorname{tr}_E = \mathbb{1} \otimes \operatorname{tr}$, where $\mathbb{1}$ is the identity map on $\mathcal{H}_S$ and tr is a trace on $\mathcal{H}_E$. In physics literature you can often find a notation*

$$\operatorname{tr}_E \rho = \sum_n \langle n|\rho|n\rangle,$$

where $\{|n\rangle\}$ is a basis of $\mathcal{H}_E$.

It is often inconvenient to have a map between two different spaces. To avoid that we fix a reference state $G = |G\rangle\langle G|$ in the environment and we define

$$\mathbb{E}[\rho] := \mathrm{tr}_E(\rho) \otimes G.$$

If we expand the trace in a basis $\{|n\rangle\}$ of $\mathcal{H}_E$ we have

$$\mathbb{E}[\rho] = \sum_n E_n \rho E_n^*, \quad E_n = \mathbb{1} \otimes |G\rangle\langle n|.$$

We defined states as density matrices, motivated by an argument of Landau that partial trace of a pure state can be a mixed (non pure) state. The following lemma shows that we were not too generous in the definition of state and that indeed all states can be obtained as partial trace of a pure state.

Lemma 4 (Purification) *Let ρ be a state on a finite dimensional Hilbert space $\mathcal{H}$. Then there exists a Hilbert space $\mathcal{H}_E$ and a pure state $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H}_E$ such that*

$$\rho = \mathrm{tr}_E |\psi\rangle\langle\psi|.$$

Proof: We write ρ in a diagonal form as $\rho = \sum_\alpha \rho_\alpha |\alpha\rangle\langle\alpha|$, where $\{|\alpha\rangle\}$ is the eigenbasis of ρ and the eigenvalues ρ_α are non-negative because ρ is a positive operator. Now choose dimension of $\mathcal{H}_E$ equal to the dimension of $\mathcal{H}$, and (with little abuse of notation) denote $\{|\alpha\rangle\}$ a basis in $\mathcal{H}_E$. Then

$$|\psi\rangle = \sum_\alpha \rho_\alpha^{1/2} |\alpha\rangle \otimes |\alpha\rangle$$

has the desired property. Indeed,

$$\mathrm{tr}_E(|\psi\rangle\langle\psi|) = \mathrm{tr}_E \left(\sum_{\alpha,\beta} \rho_\alpha^{1/2} \rho_\beta^{1/2} |\alpha\rangle\langle\beta| \otimes |\alpha\rangle\langle\beta| \right)$$

$$= \sum_\alpha \rho_\alpha |\alpha\rangle\langle\alpha| = \rho.$$

$\square$

Time evolution

The evolution of the full system $S \vee E$ is generated by a Hamiltonian and for a fixed time t the evolution from time zero to t is given by a map

$$|\psi\rangle \to U|\psi\rangle,$$

or as an operation on states

$$\rho \to U\rho U^*,$$

where U is a unitary operator. What kind of evolution this generates on S alone? This question is well defined only if we specify an initial state, the most natural choice is $\rho \otimes G$. We compute,

$$
\begin{aligned}
\mathbb{E}[U\rho \otimes GU^*] &= \sum_n E_n U\rho \otimes GU^* E_n^* \\
&= \sum_n \tilde{K}_n \rho \otimes G\tilde{K}_n^*, \quad \tilde{K}_n := E_n U.
\end{aligned}
$$

Now define an operator on $\mathcal{H}_S$ alone by

$$
(K_n|\psi\rangle) \otimes |G\rangle = \tilde{K}_n(|\psi\rangle \otimes |G\rangle),
$$

then we have

$$
\operatorname{tr}_E(U\rho \otimes GU^*) = \sum_n K_n \rho K_n^*. \tag{4}
$$

We shall see later that operators K_n that can be obtained from this construction can be arbitrary apart from a normalization condition

$$
\begin{aligned}
\sum_n \tilde{K}_n^* \tilde{K}_n &= \sum_n U^* E_n^* E_n U \\
&= \sum_n U^* \mathbb{1} \otimes |n\rangle\langle G|\mathbb{1} \otimes |G\rangle\langle n|U = \mathbb{1}.
\end{aligned}
$$

The type of map encountered on the RHS of the Eq. (4) is called Kraus map and we will see that in some sense (to be defined precisely soon) it is the most general operation allowed in quantum mechanics. We will also see that any operation of this type can be expressed as a partial trace of a unitary evolution on a system $S \vee E$.

Remark 5 *Above we chose $\rho \otimes G$ as an initial state. A general choice of an initial state can be encoded in a map $\rho \to \rho_{\bar{S}}$ such that $\operatorname{tr}_E \rho_{\bar{S}} = \rho$. If this map is linear the conclusions remain valid. In explicit there are are operators K_α such that*

$$
\operatorname{tr}_E(U\rho_{\bar{S}}U^*) = \sum_\alpha K_\alpha \rho K_\alpha^*.
$$

If the map is non-linear "anything can happen". This kind of non-linearity may occur for example in a control theory or the Hartree-Fock approximation.

2 Statistical structure of quantum theory

A full description of a measurement refers to an open system consisting (at least[1]) out of the system itself and the measuring apparatus. Hence it is of no surprise that mathematical structures encountered in the theory of measurements play a central role also in the

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[1]Some insist in including the experimentalists, others even many copies of her in many different worlds.

theory of open systems. Historically these mathematical structures were first developed into a fully consistent theory in the theory of measurements.

Statistics of measurement outcomes in any physical theory is described by a state of the system and a set of observables. An observable corresponds to a quantity that can be potentially measured on the system. A state attaches to each observable a statistics of its measurement outcomes. Both states and observables are mathematical constructs that aim to describe the reality, and often there are several equivalent descriptions of the same system.

Definition 6 (Algebraic data specifying a quantum system S) *We associate the system to a Hilbert space $\mathcal{H}_S$;*

1. *Set of observables is a subset $\mathcal{A}_S \subset \mathcal{B}(\mathcal{H}_S)$ of self-adjoint operators*

2. *Convex set of states $\mathcal{S}_S$ is formed by positive, normalized operators*

$$\mathcal{S}_S = \{\rho \in \mathcal{B}(\mathcal{H}_S) | \rho \geq 0, \operatorname{tr}\rho = 1\}$$

3. *Time evolution is specified by a map*

$$\Phi_t : \mathcal{S}_S \to \mathcal{S}_S$$

Much more careful and precise discussion can be found in [9], this paper is also an excellent exposition of fundamental problems of measurement in quantum mechanics.

Description of time evolution

We start by discussing the time evolution. More precisely we fix time t, write $\Phi \equiv \Phi_t$ and discuss general requirements imposed on Φ by principles of QM and probability. This is often called operational approach. We shall require the following

(R1) Linearity, $\quad \Phi(\alpha\rho + \sigma) = \alpha\Phi(\rho) + \Phi(\sigma)$

(R2) Trace preserving, $\quad \operatorname{tr}\Phi(\rho) = \operatorname{tr}\rho$

(R3) Complete positivity (CP-map)

The last point is explained in the following definition,

Definition 7 (Complete Positivity) *Let Φ be a map on $\mathcal{B}(\mathcal{H})$ then we say that,*

- Φ *is positive if for all $\rho \geq 0$, $\Phi\rho \geq 0$,*

- Φ *is n-positive if $\Phi \otimes \mathbb{1}_n$ acting on $\mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathbb{C}^n)$ is positive,*

- Φ *is completely positive if it is n-positive for all $n \in \mathbb{N}$.*

Sometimes requirements are justified by a theorem. This is not completely the case, but anyway let us postpone their discussion after we prove that the map satisfying this requirements is always of the form Eq. (4). This is one of the most important structural theorems in the theory of open systems.

Theorem 8 (Kraus '71) *Suppose that Φ is a map on $\mathcal{B}(\mathcal{H}_S)$ that satisfies (R1)-(R3). Then there exists a Hilbert space $\mathcal{H}_E$ a reference state G and a unitary U acting on $\mathcal{H}_S \otimes \mathcal{H}_E$ such that*

$$\Phi\rho = \mathrm{tr}_E(U\rho \otimes GU^*). \tag{5}$$

In particular there exists operators K_α with $\sum_\alpha K_\alpha^* K_\alpha = 1$ such that

$$\Phi\rho = \sum_\alpha K_\alpha \rho K_\alpha^*. \tag{6}$$

Proof: We know that (5) $\implies$ (6). We are going to prove the converse (6) $\implies$ (5) and then (R1)-(R3) $\implies$ (6).

- (6) $\implies$ (5): Consider an operator U on $\mathcal{H}_S \otimes \mathcal{H}_E$ (dimension of $\mathcal{H}_E$ is defined implicitly) that acts as

$$U\psi \otimes |G\rangle = \sum_\alpha K_\alpha |\psi\rangle \otimes |\alpha\rangle,$$

where $\{|\alpha\rangle\}$ is a basis of $\mathcal{H}_E$. Note that U is not defined on the whole space, but only on the reference subspace. On this subspace it satisfies $||U|\psi\rangle \otimes |G\rangle|| = |||\psi\rangle \otimes |G\rangle||$ and so it can be extended to a unitary on the whole space. Furthermore,

$$\mathrm{tr}_E(U\rho \otimes GU^*) = \mathrm{tr}_E(K_\alpha \rho K_\beta^* \otimes |\alpha\rangle\langle\beta|)$$
$$= \sum_\alpha K_\alpha \rho K_\alpha^* \otimes G,$$

which is the desired property.

- (R1)-(R3) $\implies$ (6): Take $\dim \mathcal{H}_E = \dim \mathcal{H}_S$. We shall use an observation of Choi that all information about Φ is encoded in a state

$$\sigma := (\Phi \otimes 1)(|\varphi\rangle\langle\varphi|), \quad \text{where} \quad |\varphi\rangle = \sum_\alpha |\alpha\rangle \otimes |\alpha\rangle,$$

for some basis $\{|\alpha\rangle\}$ of $\mathcal{H}_S$ and $\{|\alpha\rangle\}$ of $\mathcal{H}_E$. In fact $\sigma = \sum_{\alpha,\beta} \Phi(|\alpha\rangle\langle\beta|) \otimes |\alpha\rangle\langle\beta|$ and

$$(1 \otimes |G\rangle\langle\tilde{\psi}|)\, \sigma\, (1 \otimes |\tilde{\psi}\rangle\langle G|) = \sum_{\alpha,\beta} \Phi(|\alpha\rangle\langle\beta|)\langle\tilde{\psi}|\alpha\rangle\langle\beta|\tilde{\psi}\rangle \otimes G.$$

If we now pick $|\tilde{\psi}\rangle$ in such a way that $\langle\tilde{\psi}|\alpha\rangle = \langle\alpha|\psi\rangle$ we get

$$(1 \otimes |G\rangle\langle\tilde{\psi}|)\, \sigma\, (1 \otimes |\tilde{\psi}\rangle\langle G|) = \Phi(|\psi\rangle\langle\psi|) \otimes G,$$

which is the announced encoding.

The state σ is positive due to the assumption of complete positivity of Φ and we can write it as $\sigma = \sum_i |s_i\rangle\langle s_i|$. Define a linear map

$$\tilde{K}_i |\psi\rangle \otimes |G\rangle = (1 \otimes |G\rangle\langle\tilde{\psi}|)|s_i\rangle.$$

Then

$$\tilde{K}_i |\psi\rangle\langle\psi| \otimes G\tilde{K}_i^* = \sum_i (1 \otimes |G\rangle\langle\tilde{\psi}|)|s_i\rangle\langle s_i|(1 \otimes |\tilde{\psi}\rangle\langle G|)$$
$$= (1 \otimes |G\rangle\langle\tilde{\psi}|)\, \sigma\, (1 \otimes |\tilde{\psi}\rangle\langle G|) = \Phi(|\psi\rangle\langle\psi|) \otimes G.$$

As usual we can "erase" G from above equations and redefine K_i accordingly to finish the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Let me end the section with a small discussion of (R1)-(R3). Property (R2) represents conservation of probability. Quantum mechanics is fundamentally linear (R1), however you can encounter non-linear evolutions in certain approximative many body methods like the Hartree-Fock theory. Complete positivity (R3) is connected to the existence of entangled states, if the system under consideration might be entangled with an auxiliary system then (R3) is required. I am not aware of any evolution used in QM theory for which (R3) would not be true. To sum up the discussion (R1)-(R3) should be expected if the evolution describes an experiment in which general initial state is transformed by the apparatus to some final state.

Description of measurement

We follow a book of Holevo [12]. There are three levels of description of a measurement,

1. Probability of measurement outcomes (only),

2. Law of transformation; Posterior state,

3. Full Dynamics

Statistical structure of quantum mechanics gives framework of the first two points, point 3 belongs to the realm of fully Hamiltonian descriptions of the system and the environment.

Let us first consider the case of an operator with a discrete spectrum, $A = \sum a_j P_j$, where P_j are finite dimensional orthogonal projections that decompose the identity, i.e.

$$P_j^2 = P_j, \quad P_j P_k = 0 \quad \text{for} \quad (j \neq k), \quad \sum P_j = 1.$$

We have $<A>_\psi = \sum a_j \langle \psi | P_j | \psi \rangle$, and we see that a probability of a measurement outcome a_i is $\langle \psi | P_i | \psi \rangle$. More generally a probability that an outcome is in certain subset of possible results is given by

$$Prob(A \in E \subset \mathbb{R}) = \sum_{j : a_j \in E} \langle \psi | P_j | \psi \rangle$$

$$= \langle \psi | P_E | \psi \rangle, \quad P_E = \sum_{j : a_j \in E} P_j.$$

A map $E \to P_E$ maps a subset of $\mathbb{R}$ into a projection, which in turn determines a probability (measure) by the above rule. The map is an example of a projection operator valued measure, a name often shortened as POVM. We will see that in general POVM is an appropriate framework for description of the item 1.

The statistics of measurement outcomes was described in terms of the wave function $|\psi\rangle$. If only the statistics of outcomes is required one does not need to use the notion of a state in order to have a self-contained theory. For the full theory of measurement the

notion of state is essential. For a state ρ the probability of a measurement outcome being in the set E is given by

$$Prob(A \in E \subset \mathbb{R}) = \text{tr}(P_E \rho),$$

where P_E has the same meaning as in the paragraph above. In particular for an average of an observable A we have

$$<A>_\rho = \text{tr}(A\rho).$$

Notice that these formulas coincide with the corresponding formulas in the preceding paragraph if $\rho = |\psi\rangle\langle\psi|$.

As of item 2., for a discrete observable A, the posterior state given outcome a_j is

$$\rho_j = \frac{P_j \rho P_j}{Prob(x_j)}.$$

And the posterior state given $x \in E$ is

$$\rho_E = \frac{\sum_{x_j \in E} P_j \rho P_j}{Prob(x \in E)} = \frac{\mathcal{E}_E(\rho)}{p(E)},$$

where $\mathcal{E}_E$ is a CP map that can be red of from the equality. The map $E \to \mathcal{E}_E$ is called an *instrument* and it is an appropriate framework for description of the item 2.

The formula for posterior state is usually derived in QM classes using repeatability hypothesis: "If the physical quantity is measured twice in succession in a system S we get the same value each time". In explicit, the probability that the measurement outcome is in the set E given state ρ_E is equal to 1. This is indeed so,

$$\text{tr}(\mathcal{E}_E(\rho)P_E) = \text{tr}(\sum_{x_j \in E} P_j \rho P_j P_E) = \text{tr}(\rho P_E) = p(E),$$

and hence $\text{tr}(\rho_E P_E) = 1$. We will see that this hypothesis fails in the case of a general observable.

The general case. In infinite dimensions there is no analog for the probability of a single outcome, however probability of outcome being in a certain region is well defined. To each self adjoint operator A there correspond a unique orthogonal POVM P_E such that the probability of the measurement outcome being in a set E is given by $\langle \psi | P_E | \psi \rangle$. The projection P_E is related to A by means of a spectral calculus $P_E = \chi_E(A)$, χ_E being a characteristic function of a region E. The spectral decomposition of A is often written in a form

$$A = \int_{\mathbb{R}} a \, P(\text{d}a)$$

and P_E is then given by $P_E = \int_E P(\text{d}a)$.

This accomplishes description of item 1. for a general observable. There is no analog to item 2. The obstruction is the uncertainty principle. Upon measuring position the "posterior state" is a delta function, which is a non-normalizable state with an infinite energy. In what follows we describe the general framework for items 1 and 2.

Statistics of measurement outcomes

The statistics of measurement outcomes is described by a POVM (projection operator valued measure). Suppose $\mathcal{M}$ is the space of measurement outcomes then a map

$$E \subset \mathcal{M} \quad \rightarrow \quad \Pi(E) \in \mathcal{B}(\mathcal{H})$$

is called POVM if

i) $\Pi(E) \geq 0$,

ii) $\Pi(E_1 \bigcup E_2) = \Pi(E_1) + \Pi(E_2)$ provided $E_1 \bigcap E_2 = 0$,

iii) $\Pi(\mathcal{M}) = 1$.

The probability of a measurement outcome a given state ρ is then associated to a POVM by a relation

$$Prob(a \in E) = \text{tr}(\Pi(E)\rho).$$

Conditions i) to iii) guarantees that this is indeed a probability distribution.

Law of transformation

The law of transformation is described by an *instrument*. This is a map

$$E \subset \mathcal{M} \quad \rightarrow \quad \mathcal{E}_E$$

such that

i) $\mathcal{E}_E$ is a CP map on $\mathcal{B}(\mathcal{H})$,

ii) $\mathcal{E}_{E_1 \bigcup E_2} = \mathcal{E}_{E_1} + \mathcal{E}_{E_2}$ provided $E_1 \bigcap E_2 = 0$,

iii) $\mathcal{E}_{\mathcal{M}} = 1$.

Given a measurement outcome $a \in E$ the state of the system is transformed according to $\rho \rightarrow \mathcal{E}_E(\rho)/p(E)$. The normalization gives $p(E) = \text{tr}\,\mathcal{E}_E(\rho) = \text{tr}(\rho\mathcal{E}_E^*(\mathbb{1}))$. For each instrument there is a unique POVM $\Pi(E) = \mathcal{E}_E^*(\mathbb{1})$ that gives statistics consistent with the law of transformation. The converse is not true, for each POVM there are infinitely many instruments that gives that particular statistics.

More physical discussion of the latter statement might be helpful at this place. Imagine you want to measure the z-component of a spin. For this purpose you set up a Stern-Gerlach type experiment in which the spin traverse through a region of an in homogenous magnetic field pointing in the z-direction and measure proportion of spins seeking low/high magnetic field. It is completely plausible that the spin traverse through further magnetic field in general directions before leaving your measuring apparatus. The posterior state will depend on this additional magnetic fields, however the proportion of low/high field seekers will be independent of it.

Historically people tried to assign to each POVM a unique "minimal" instrument with the help of the repeatability hypothesis. It turned out that for continuous observables such instruments simply does not exist and the general theory does not refer to this hypothesis anymore. In the case of the above Stern-Gerlach type experiment the repeatability hypothesis would single out an apparatus without any additional magnetic fields.
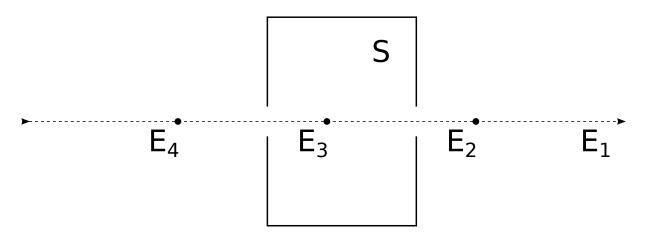
Figure 1: Sketch of the repeated interaction model. The environment E_3 interacts with the system S only for times $3T \leq t \leq 4T$.

3 Hamiltonian Approach

This is the most fundamental approach to open quantum systems. We solve Schrödinger equation on the joint system $S \vee E$ and obtain the state on S by taking the partial trace. An explicit solution of the joint Schrödinger equation is known only for a very few systems, and we shall study a particular example called *repeated interaction model*. On one hand this provides us with a case study of an open quantum system, on the other hand it describes recent experiments of Haroche. To go a step beyond explicit solutions, in Section 5 we will study dynamics of large class of models in a well control approximation of a small coupling between the system and the bath.

Repeated interaction model

In repeated interaction model the environment is composed of independent subsystems called probes, $E = \vee_{j=0}^{\infty} E_j$, which successively interact with the system S (see figure 3.). The probe E_n interacts with the system only for a time T during the time interval $(nT, (n+1)T)$. This assumption simplifies the notation, generalization to the case when there is a dead time between interaction of E_n and E_{n+1} with S is straightforward.

Instead of describing the free evolution of the n-th probe for $0 \leq t \leq nT$ we assume that at the onset of the interaction the probe is in the state G_n and that it is uncorrelated with the system and the remaining probes. The free dynamics of the system and the probe is described by a Hamiltonian H_0, the interaction between the system and the $n-th$ probe by a (in general time dependent) Hamiltonian H_n. If $\rho(nT)$ is the state of S at time nT then the time evolution of $S \vee E_n$ is given by

$$\rho_{S \vee E_n}(nT + \tau) = U_n(\tau)\rho(nT) \otimes G_n U_n^*(\tau), \quad , 0 \leq \tau \leq T,$$

$$U_n(\tau) := \text{Texp}(-i(\int_0^\tau H_0 + H_n(s))).$$

It follows in particular that the state of the system at the time when the $(n+1)$-th probe

begins to interact is

$$\rho((n+1)T) = \mathrm{tr}_{E_n} U_n(T)\rho(nT) \otimes G_n U_n^*(T) =: \Phi_n(\rho(nT)),$$

where Φ_n is the associated Kraus map obtained by taking the partial trace. For the dynamics of the system from time 0 until time $t = nT + \tau$, $0 \le \tau \le T$ with an initial condition $\rho(0)$ we then have,

$$\rho(t) = \mathrm{tr}_{E_n} U_n(\tau)(\Phi_{n-1} \ldots \Phi_0 \rho(0))U_n^*(\tau).$$

The formula further simplifies if we assume that all probes are (distinguishable) copies, i.e. $E_j \simeq E_k$ and given this identification $G_j \simeq G_k$, $U_j \simeq U_k$. It then follows that $\Phi_j = \Phi_k$ (Notice that no identification is needed here as Φ_k operates only on S) and dropping indices in Φ, G etc we get

$$\rho(t) = \mathrm{tr}_E U(\tau)(\Phi^n \rho(0))U^*(\tau),$$

or at the multiples of the interaction time T, $\rho(nT) = \Phi^n \rho(0)$.

Long time properties of the evolution are determined by the map Φ. For example if Φ has a unique stationary state and $\sigma(\Phi) \setminus \{0\} \in B_{1-\varepsilon}$ then $\rho(nT) \to \sigma$. In the following we shall work out Φ for two special cases.

Dephasing case

For concreteness we assume that probes are two level systems and that the spectrum of the free Hamiltonian is non degenerate with eigenbasis $|n\rangle \otimes |\pm\rangle$. Suppose that the interaction Hamiltonian is time independent and that it commutes with the free Hamiltonian. Then we have

$$(H_0 + H_1)|n\rangle \otimes |\pm\rangle = E_{n,\pm}|n\rangle \otimes |\pm\rangle.$$

We can also define an effective Hamiltonian of the system given that probe is in the $+$ or $-$ state,

$$H_+ = \sum E_{n,+}|n\rangle\langle n|, \quad H_- = \sum E_{n,-}|n\rangle\langle n|.$$

The time evolution in terms of these two Hamilotnians is

$$e^{-i(H_0+H_1)\tau}|\psi_S\rangle \otimes (c_-|-\rangle + c_+|+\rangle) = c_- e^{-i\tau H_-}|\psi_S\rangle \otimes |-\rangle + c_+ e^{-i\tau H_+}|\psi_S\rangle \otimes |+\rangle.$$

From this expression we can read the associated Kraus map,

$$\Phi(\rho) = |c_-|^2 U_- \rho U_-^* + |c_+|^2 U_+ \rho U_+^*, \quad U_\pm = e^{-iTH_\pm}.$$

By construction this is a dephasing Kraus map, all spectral projections $|n\rangle\langle n|$ are stationary. We want to find conditions under which an initial coherent superposition of $|n\rangle$ and $|m\rangle$ approaches an incoherent mixture of these states. In other words when $|n\rangle$, $|m\rangle$ is distinguishable by the apparatus. We have

$$\Phi(|n\rangle\langle m|) = \lambda_{nm}|n\rangle\langle m|, \quad \lambda_{nm} = |c_-|^2 e^{-i(E_{n,-}-E_{m,-})T} + |c_+|^2 e^{-i(E_{n,+}-E_{m,+})T}.$$

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It is now easy to give conditions under which $|\lambda_{nm}| < 1$. A trivial condition is that both c_+ and c_- need to be nonzero. If, for example, $c_- = 0$ then $|\lambda_{mn}| = 1$ for any choice of interaction Hamiltonian.

There is further condition on the interaction energy. To describe this condition we write $E_{n,\pm} = E_{n,\pm}^{(0)} + E_{n,\pm}^{int}$, where $E^{(0)}$, E^{int} is the contribution from H_0 and H_1 respectively. The free energy $E^{(0)}$ is a sum of the energy of the system and the probe and hence $E_{n,+}^{(0)} - E_{n,-}^{(0)}$ is independent of n. The condition is then expressed in terms of $\Delta E_n^{int} = E_{n,+}^{int} - E_{n,-}^{int}$,

$$(\Delta(E_n^{int}) - \Delta(E_m^{int}))T = 0 \quad \mod 2\pi. \tag{7}$$

Experiment of Haroche

If you want to read some original articles about these Nobel winning experiments you can take a look for example at [6, 11].

S: Cavity with an electro magnetic field; High Q cavity with the life time of photon around 100μs.

E: Rubidium atom in a circular Rydberg state with a principal quantum number $n = 50, 51$.

Rydberg atoms are used thanks to their strong dipole interaction and long radiative lifetime, around 30ms. Rubidium has a simple electron structure and can be easily ionized because it has a 1 electron in its shell (it is an alkali metal).

We consider a subspace of zero angular momentum and denote by $|g\rangle$ the state with principle number $n = 50$ and by $|e\rangle$ the state with the principal number $n = 51$. The atoms are prepared in such a way that they enter the cavity in certain superposition of ground and excited state. For simplicity we shall consider an equal superposition

$$|G\rangle \equiv \frac{1}{\sqrt{2}}(|e\rangle + |g\rangle).$$

Interaction of a mode a of the electro magnetic field in the cavity with the atom is described by the Jaynes-Cummings Hamiltonian

$$H = \omega_c(a^*a + \frac{1}{2}) + \omega_0\frac{\sigma_z}{2} + \frac{\Omega}{2}f(x)(a^*\sigma_- + a\sigma_+),$$

where ω_c is the frequency of the cavity mode, ω_0 is the frequency of the transition e to g and Ω is the dipole interaction. $\sigma_\pm$ are raising operators, e.g. $\sigma_-|e\rangle = |g\rangle$. Space dependent function f represents varying strength of the interaction inside the cavity, it vanishes in the boundary and attains its maximum in the center of the cavity. The parameter x represents the position of the Rubidium atom, for an atom flying at a constant speed v we can write $x = vt$. This substitution makes the Hamiltonian time dependent.

An important parameter of the model is the detuning $\delta = \omega_c - \omega_0$. If $\delta/\Omega \simeq 0$ the atom and the field are in resonance, when $|\delta/\Omega| >> 0$ then the atom and the field are off-resonant. The experiments of Haroche are in the off-resonant regime, $\delta = 300$kHz and $\Omega = 50$kHz. Note that ω_c is tunable by changing the cavity geometry.

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We want to solve the time-dependent Schrödinger equation describing the atom-cavity interaction. The solution can be derived using the adiabatic theory, which is described in some details below.

Before entering the cavity $t < 0$ and after leaving the cavity $t > T$ we have $f = 0$ (which is the same as $\Omega = 0$) and $\delta \neq 0$ the eigenstates of the Hamiltonian are $|n, g\rangle$ and $|n, e\rangle$ with energies

$$H|n, g\rangle = (\omega_c(n + 1/2) - 1/2\omega_0)|n, g\rangle, \quad H|n, e\rangle = (\omega_c(n + 1/2) + 1/2\omega_0)|n, e\rangle.$$

Inside the cavity the eigenstates and eigen-energies depend continuously on time if we stay in a off-resonant case. We denote the eigen-energies by $E_{(n,g)}(t)$ and $E_{(n,e)}(t)$. By the adiabatic theorem we know that

$$|\psi(T)\rangle = \frac{1}{\sqrt{2}}(e^{-i\int_0^T E_{(n,g)}(t)\mathrm{d}t}|n, g\rangle + e^{-i\int_0^T E_{(n,e)}(t)\mathrm{d}t}|n, e\rangle)$$

is the solution of the Schrödinger equation with the initial condition $|\psi(0)\rangle = |G\rangle \otimes |n\rangle$ up to an small error that we address in the next paragraph. This is exactly of the same type as the dephasing case. In the experiment of Haroche the accumulated phase was equal to $\frac{n\pi}{8}$. In particular the experiment can distinguish number of photons modulo 8.

A dimensionless small parameter that characterize error in the adiabatic approximation is

$$\varepsilon \sim ||\dot{H}||/g^2 \sim \frac{\Omega}{\delta^2 T}.$$

It is of order 10^{-1} in the experiment of Haroche. If the error is of order ε as suggested by the adiabatic theorem then this is a bad sign. On the other hand if we believe that the error is of order $\exp(-\varepsilon^{-1})$ as suggested by the Landau-Zener formula then is a good sign. The theory does not give any comprehensive answer but experience suggest that Landau-Zener type scaling is more appropriate. In other words adiabatic approximation is very good already for the adiabatic parameter of order 0.1. In this case it is not hard to do computer simulations and they showed that the error is indeed negligible.

Let us summarize, Haroche realized a repeated interaction model in which

$$|n\rangle \otimes |\pm\rangle \quad \rightarrow \quad e^{\Phi_{\pm}(n)}|n\rangle \otimes |\pm\rangle, \quad \Phi_{\pm}(n) = \pm\frac{n\pi}{8}.$$

We shall se in Section **??** how this can be used to measure the number of photons in the cavity modulo 8.

Adiabatic evolution in quantum mechanics

We will derive solutions to a slowly driven Schrödinger equation

$$i|\dot{\psi}(t)\rangle = H(\varepsilon t)|\psi(t)\rangle. \tag{8}$$

The equation represents separation of scales in the system with a ratio of the slow scale to the fast scale equal to ε. The physical origin of the splitting slow/fast vary. In quantum control or quantum adiabatic computation it is an externally applied slow driving,

the small parameter ε being tuned by the experimentalists. In Born-Oppenheimer approximation (8) is a Hamiltonian of electrons for a slow motion of heavy nuclei, ϵ being determined by electron to proton mass ratio. In the experiment of Haroche that we are going to discuss it is a description of a particle slowly flying through an inhomogeneous external field.

Solutions of (8) can be expanded as an asymptotic series in ε provided the energy levels of the Hamiltonian do not cross. The latter requirement is traditionally rephrased as the gap condition. In terms of the Hamiltonian eigendecomposition

$$H(\varphi) = \sum E_j(\varphi)|\psi_j(\varphi)\rangle\langle\psi_j(\varphi)|,$$

we say that $H(\varphi)$ satisfies a gap condition if

$$|E_j(\varphi) - E_k(\varphi)| > 0 \quad \forall\varphi \quad \text{and} \quad j \neq k.$$

Theorem 9 (Adiabatic theorem) *Suppose that $H(\varphi)$ satisfies the gap condition. Then the solution of the Schrödinger equation (8) with an initial condition $|\psi(0)\rangle = |\psi_j(0)\rangle$ is*

$$|\psi(t)\rangle = e^{-i\frac{1}{\varepsilon}\varphi_d(t)+i\varphi_b(t)}|\psi_j(\varepsilon t)\rangle + o(\varepsilon),$$

where the dynamical phase

$$\varphi_d(t) = \int_0^{\varepsilon t} E_j(\varphi)\mathrm{d}\varphi,$$

and the Berry phase

$$\varphi_b(t) = i \int_0^{\varepsilon t} \langle\psi_j(\varphi)|\dot{\psi}_j(\varphi)\rangle\mathrm{d}\varphi.$$

The theorem provides no quantitative information about the error $o(\varepsilon)$. Even though a bound on the error of the form $\varepsilon\|\dot{H}\|/g^2$ where g is the gap in the spectrum can be derived, it is typically very pessimistic. For a smooth compactly supported change the Landau-Zener formula (discussed below) tends to be more precise.

Two level crossing

When two eigenenergies of a system collide at certain time we speak about a (energy) level crossing. Without loss of generality we can assume that it occurs at time $s = 0$ at energy $E = 0$. Zooming into this point and keeping only the linear terms, the energy difference between the levels is linear with a slope ε,

$$E_0(t) - E_1(t) = \varepsilon t$$

and the Hamiltonian in an appropriate basis is a two by two matrix

$$H(t) = \frac{1}{2}\begin{pmatrix} \varepsilon t & 0 \\ 0 & -\varepsilon t \end{pmatrix}.$$

A generic interaction between these two energy levels would lift the degeneracy at $t = 0$. The Hamoltonian with a real interaction is

$$H(t) = \frac{1}{2}\begin{pmatrix} \varepsilon t & g \\ g & -\varepsilon t \end{pmatrix}. \tag{9}$$
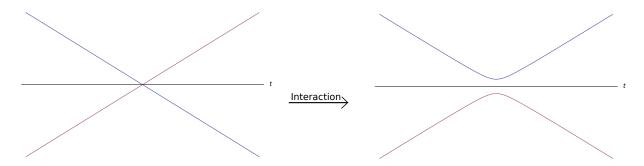
Figure 2: Energy of two levels depending on time. A generic Interaction lifts an energy level crossing into an avoided crossing

and the energy difference is

$$E_0(t) - E_1(t) = \sqrt{\varepsilon^2 t^2 + g^2}.$$

The minimum energy difference, called gap, is at $t = 0$ and equal to g. This is called an avoided crossing (see figure 3).

As a rule of thumb all crossings that are not protected by a symmetry are avoided crossings.

Landau-Zener formula

Consider the Hamiltonian (9) and its two eigenstates

$$H(t)|\psi_0(t)\rangle = E_0(t)|\psi_0(t)\rangle, \quad H(t)|\psi_1(t)\rangle = E_1(t)|\psi_1(t)\rangle.$$

Let $|\psi(t)\rangle$ be a solution of the Schrödinger equation $i|\dot{\psi}(t)\rangle = H(t)|\psi(t)\rangle$ with an initial condition $|\psi(-\infty)\rangle = |\psi_0(-\infty)\rangle$. Then the probability to find the state in the excited state at $t = \infty$ is given by the Landau-Zener formula

$$|\langle\psi(\infty)|\psi_1(\infty)\rangle|^2 = e^{-\pi g^2/2\varepsilon}.$$

For the Hamiltonian (9) this is an exact formula. For adiabatic crossing only the shape of the crossing matters and the formula holds in the leading order as $\varepsilon \to 0$ irrespectively of how exactly the Hamiltonian looks like for $|t| >> 0$ (provided there are no other energy crossings).

Note that ε in the Hamiltonian (9) is not dimensionless. To compare it with the adiabatic theorem you might want to introduce a dimensionless units. This is left as an exercise.

4   Markovian master equation

The term master equation refers to a large class of physical models that effectively, and often probabilisticly, describe evolution of some degrees of freedom in a closed form. In classical mechanics the prime example is the Fokker-Planck equation describing evolution of a Brownian particle under influence of drag forces.

In connection to open quantum systems master equations describe evolution of the system alone. This is of major importance in basically all realistic situations when solving for the join system-environment evolution is intractable, or when the join Hamiltonian is not even known.

Markovian master equations describe systems coupled to memoryless environments. The theory of such equations was developed by Davies, Lindblad and Kossakowski et. al. In particular the general form of the generator of the evolution was derived. This form is referred to as Lindblad equation, the main part of this section is a proof of this result.

A master equation of a Lindblad form for the state of the system $\rho(t)$ has a form

$$\dot{\rho}(t) = L\rho(t)$$

with a Lindblad generator

$$L\rho = -i[H, \rho] + \sum_\alpha 2\Gamma_\alpha \rho \Gamma_\alpha^* - \Gamma_\alpha^* \Gamma_\alpha \rho - \rho \Gamma_\alpha^* \Gamma_\alpha, \tag{10}$$

where $H = H^*$ and Γ_α are arbitrary operators. Using a completely positive map $\Phi(\rho) = 2\sum \Gamma_\alpha \rho \Gamma_\alpha^*$ this can be equivalently written as

$$L\rho = -i[H, \rho] + \Phi(\rho) - \frac{1}{2}(\Phi^*(\mathbb{1})\rho + \rho\Phi^*(\mathbb{1})).$$

Lindblad equation in its general form was first derived by Davies in a study of continuous measurements. We give the basic idea and describe a process in which the system is measured in random times with frequency γ. Let $\Phi(\cdot)$ be a Kraus map with $\Phi^*(\mathbb{1}) = \mathbb{1}$ that describes a transformation of the state upon a measurement. Suppose that in the time interval $\mathrm{d}t$ the state is measured with a probability $\gamma\mathrm{d}t$ and with probability $(1-\gamma\mathrm{d}t)$ the state evolves by a Hamiltonian evolution,

$$\rho(t + \mathrm{d}t) = (1 - \gamma\mathrm{d}t)e^{-iH\mathrm{d}t}\rho(t)e^{iH\mathrm{d}t} + \gamma\mathrm{d}t\Phi(\rho(t)).$$

Expanding this to the first order in $\mathrm{d}t$ we get

$$\dot{\rho}(t) = -i[H, \rho(t)] + \gamma\Phi(\rho(t)) - \gamma\rho(t),$$

which is of the Lindblad form because we have assumed that $\Phi^*(\mathbb{1}) = \mathbb{1}$.

In general, without the latter assumption, let $\Phi(\rho)$ be a completely positive map. Let the "probability" of applying this map be $0 \le \Phi^*(\mathbb{1}) \le \mathbb{1}$, then a map

$$\rho \to \sqrt{1 - \Phi^*(\mathbb{1})}\rho\sqrt{1 - \Phi^*(\mathbb{1})} + \Phi(\rho),$$

is a Kraus map that represents in the minimal way that we did nothing on the complement. It is then straightforward to generalize the argument of the previous paragraph. We consider a process in which we evolve the state by $\mathrm{d}t\Phi(\rho)$ with probability $\mathrm{d}t\Phi^*(\mathbb{1})$ and evolve by a Hamiltonian evolution otherwise,

$$\rho(t + \mathrm{d}t) = \sqrt{1 - \mathrm{d}t\Phi^*(\mathbb{1})}e^{-iH\mathrm{d}t}\rho(t)e^{iH\mathrm{d}t}\sqrt{1 - \mathrm{d}t\Phi^*(\mathbb{1})} + \mathrm{d}t\Phi(\rho(t)).$$

Expanding to the first order in $\mathrm{d}t$ then gives the Lindblad equation in its general form,

$$\dot{\rho}(t) = -i[H, \rho(t)] + \Phi(\rho(t)) - \frac{1}{2}(\Phi^*(\mathbb{1})\rho(t) + \rho(t)\Phi^*(\mathbb{1})).$$

The general form of markovian master equation

The following theorem that classifies all Markovian master equations was proved independently by Lindblad [13] and Gorini, Kossakowski, Sudarshan [10]. This is the most important structural theorem of the theory of open quantum systems.

Theorem 10 *Suppose that $\Phi_t(\cdot)$ is a family of Kraus maps such that*

(i) $\Phi_t(\cdot)$ is a trace preserving CP map,

(ii) Φ_t is a semigroup, i.e. $\Phi_{t+s}(\cdot) = \Phi_t\Phi_s(\cdot)$ holds for all $s, t > 0$,

(iii) $\Phi_t(\cdot)$ is continuous.

then the state $\rho(t) := \Phi_t\rho$ satisfies a Lindblad Eq.(10), i.e. $\Phi_t = e^{Lt}$ for some Lindbladian L.

Proof: I have followed the proof given in [15] and you can find all details there.

Example 11 (Example of Lindblad operator) *Notation: $E_{jk} = |j\rangle\langle k|, P_j = |j\rangle\langle j|, H = \sum \lambda_j P_j$. Let*

$$L\rho = -i[H, \rho] + \sum_{jk}\gamma_{jk}(2E_{jk}\rho E_{jk}^* - E_{jk}^* E_{jk}\rho - \rho E_{jk}^* E_{jk})$$

$$= -i[H, \rho] + 2\sum_{jk}\gamma_{jk}E_{jk}\rho E_{jk}^* - \sum_{jk}\gamma_{jk}(P_k\rho + \rho P_k).$$

Define

$$L_{jk} = 2\gamma_{kj}, \quad j \neq k,$$
$$L_{jj} = 2\gamma_{jj} - 2\sum_k \gamma_{kj} = -2\sum_{k \neq j}\gamma_{kj} \leq 0$$

Then

$$L(|j\rangle\langle k|) = \left[-i(\lambda_j - \lambda_k) - \gamma_{jj} - \gamma_{kk} + \frac{1}{2}L_{jj} + \frac{1}{2}L_{kk}\right]|j\rangle\langle k|, \quad j \neq k \qquad (11)$$

$$L(P_j) = \sum_k L_{jk}P_k.$$

In particular for populations $n_j = \operatorname{tr}(P_j\rho)$ we get an equation $\dot{n}_j = \sum_k n_k L_{kj}$.
  Proof: *Computation left as an exercise* □
  Remarks:

- *Conservation of probability is equivalent to $\sum_j L_{kj} = 0$ for all k.*

- *L_{kj} is a rate of $k \to j$ transition.*

- *The off-diagonal terms of the density matrix in $|j\rangle$ basis decay, cf. Eq. (11). $\gamma_{jj} + \gamma_{kk}$ is a dephasing contribution, $1/2(L_{jj} + L_{kk})$ is an emission-absorption contribution. Note that an emission-absorption implies decoherence of off diagonal elements.*

Detail balance condition: *We say that L satisfies a detail balance condition with respect to σ if*

$$\sigma_k L_{kj} = L_{jk}\sigma_j \quad holds\ for\ all \quad j,k.$$

It implies that σ_j is a stationary state and that there are no probability currents in the system. The most typical case is that of thermal equilibrium $\sigma_j = e^{-\beta E_j}$ and

$$\frac{L_{kj}}{L_{jk}} = e^{-\beta(E_j - E_k)}.$$

5 Weak coupling limit

I have followed an article of Davies [7] and took examples from a book of Rivas, Huelga [16].

6 Soft Properties

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We will discuss two notions of distance that are non-increasing under quantum operations:

1. Relative entropy

2. Bures metric

These are just two examples of a large set of such distances, it should provide you with a flavor of the subject.

Very good introduction to the notion of entropy is given in Nielsen-Chuang Chapter. In particular monotonocity of relative entropy is proven in [].

Bures Metric

In this section we study the set of states from the perspective of differential geometry. Quantum mechanics does not equip states with any geometric structures like connection or metric. Such structures arise only from particular applications, and different applications lead to different structures. Geometric view on the set of states appears for example in quantum statistics, the linear response theory or the adiabatic theory.

We consider a Hilbert space of a finite complex dimension N, so that states ρ are Hermitian, positive $N \times N$ matrices. The states of full rank form a manifold,

$$\mathcal{M} = \{\rho > 0, \operatorname{tr}\rho = 1\}.$$

$\mathcal{M}$ is homomorphic (corresponding coordinates are discussed in details in problem **??**) to an open, convex subset of $\mathbb{R}^{N^2-1}$. Hence topologically $\mathcal{M}$ is a very simple manifold. Being full rank is important because closed subsets are not manifolds, the boundary does not locally look like $\mathbb{R}^{N^2-1}$.

It will be convenient to think of ρ as a matrix without specifying particular coordinates. The tangent space $T_\rho\mathcal{M}$ at the point ρ can be represented by Hermitian matrices of zero trace. In this representation vectors are global objects in the sense that for any $T \in T_\rho\mathcal{M}$ and small enough h, $\rho + hT \in \mathcal{M}$. This is a direct consequence of being a single chart manifold.

A natural object is a matrix valued one form $\mathrm{d}\rho$, representing infinitesimal change of the state ρ. When vectors are represented by Hermitian matrices of zero trace then $\mathrm{d}\rho$ is an identity mapping,

$$\mathrm{d}\rho(T) = T, \quad T \in T_\rho\mathcal{M}.$$

This might seem to be an unnecessary complicated and incomprehensible notation, but see the box below. Anyway, if tangent spaces and forms cause you a headache, think of $\mathrm{d}\rho$ as a small change à la the standard line element $\mathrm{d}s$.

The idea that change is a form can be demonstrated on a taylor expansion of a multivariable function,

$$f(x + h) = f(x) + h \cdot \nabla f(x) + o(h^2) = f(x) + \mathrm{d}f(x)(h) + o(h^2),$$

where we defined a one form $\mathrm{d}f(x)$ by $\mathrm{d}f(x)(h) := h \cdot \nabla f(x)$. The change of f depends on the direction, hence the first order term in the Taylor expansion gives the change as a function of the vector h.

Now we equip $\mathcal{M}$ with a metric relevant to quantum statistics. The Bures metric g at a point ρ is given by

$$g = \mathrm{tr}(\rho(A_\rho^{-1}\mathrm{d}\rho)^2),$$

where $A_\rho \cdot = \{\rho, \cdot\}$ is an anticommutator. For a curve $\rho(\varphi)$ the square of the length element associated to this metric is called Fisher information,

$$F(\varphi) := g(\dot{\rho}(\varphi), \dot{\rho}(\varphi)) = \mathrm{tr}(\rho(\varphi)(A_{\rho(\varphi)}^{-1}\dot{\rho}(\varphi))^2).$$

In connection to the quantum estimation theory, the Fisher information is interpreted as distinguishability of neighboring states. One concrete demonstration is the following. Imagine that $\rho(\varphi)$ is an output state of an interferometric device and our aim is to determine the angle φ by a measurement. Let $\hat{\varphi}$ be an estimate of the value of ϕ based on the measurement outcome. Since the measurement outcome is random, $\hat{\varphi}$ is random and its precision can be measured by its variance. Cramer-Rao bound [4] gives a universal bound (that can also be achieved) on this variance,

$$\mathbb{E}[(\varphi - \hat{\varphi})^2] \geq \frac{1}{F(\varphi)}.$$

The bigger Fisher information the better you can estimate the value of φ.

It is a natural property of information that you cannot increase it by post processing. This is reflected by monotonicity of the Bures metric and Fisher information under quantum operations.

Theorem 12 *Consider a positive, trace preserving map (Kraus map) Φ and let $F(\varphi)$ (resp. $F_\Phi(\varphi)$) be the Fisher information associated to the family of states $\rho(\varphi)$ (resp. $\Phi\rho(\varphi)$). Then it holds*

$$F(\varphi) \geq F_\Phi(\varphi).$$

Proof: Fisher information can be expressed as a maximum of the following quadratic functional,

$$F(\varphi) = sup_X \, \text{tr}\left(-X^2\rho(\varphi) + 2X\rho'(\varphi)\right), \quad X = X^*.$$

We then have

$$\begin{aligned}
F(\varphi) &\geq sup_X \, \text{tr}\left(-\Phi^*(X)^2\rho(\varphi) + 2\Phi^*(X)\rho'(\varphi)\right)\\
&\geq sup_X \, \text{tr}\left(-\Phi^*(X^2)\rho(\varphi) + 2\Phi^*(X)\rho'(\varphi)\right)\\
&= sup_X \, \text{tr}\left(-X^2\Phi\rho(\varphi) + 2X\Phi\rho'(\varphi)\right) = F_\Phi(\varphi),
\end{aligned}$$

where in the second step we used an inequality $\Phi^*(X^2) \geq \Phi^*(X)^2$. $\qquad\square$.

Example 13 (Bures metric for Qbit) *In the standard Bloch parameterization of states $\rho = (\mathbb{1} + n \cdot \sigma)/2$ with $|n| < 1$, the Bures metric is*

$$g = \frac{dn^2}{4} + \frac{1}{4}\frac{(n \cdot dn)^2}{1 - n^2}.$$

In the spherical coordinates $n = r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ it is given by

$$g = \frac{1}{4}\left(\frac{1}{1-r^2}dr^2 + r^2 d\Omega^2\right),$$

where Ω is the spherical surface element.

Proof: *To find the metric we need to solve an anti-commutator equation*

$$\left\{\frac{\mathbb{1} + n \cdot \sigma}{2}, dX\right\} = \frac{dn \cdot \sigma}{2}$$

and the metric is then given by $g_\rho = \text{tr}(\rho dX^2)$. Writing $dX = dx_0 + dx \cdot \sigma$ we have $g = dx_0^2 + dx^2 + 2dx_0 dx \cdot dn$ and the equation is equivalent to equations

$$dx_0 + n \cdot dx = 0, \quad 2dx + 2dx_0 n = dn.$$

If you express dn^2 from the second equation and then solve for dx_0 from the first equation you obtain the first form of the metric.

Changing to spherical coordinates is standard. $\qquad\square$.

Note that the metric becomes singular when you approach pure states, i.e. $|n| \to 1$. If we, however, restrict ourselves to spherical directions the metric approaches the standard Euclidean metric on the sphere up to the factor $1/4$.

7 Stochastic quantum equations

External classical parameters that determine the time evolution of a quantum system often change in time in a non-deterministic[2] way. Here we describe the situation when the unknown parameter $b(t)$ can be described as a realization of a stationary random process. This is the case when long time averages match statistical averages e.g.

$$\frac{1}{T} \int_0^T b(t+h)b(t)\mathrm{d}t = \mathbb{E}[b(h)b(0)],$$

an assumption known as the ergodic hypothesis.

Physical examples of such a parameter are voltage in the socket, field of a laser, magnetic field or more or less any other external potential. To be specific we consider the most simple example of a spin in an external field with the Hamiltonian

$$H = \omega \sigma_z(1 + b(t)).$$

Solutions of the corresponding Schrödinger equations are random objects and we aim to determine their statistics.

The random parameter $b(t)$ appears in the Hamiltonian only as a multiplicative factor. This is a tremendous simplification and the equation is exactly solvable. We write $|\psi\rangle = c_+|+\rangle + c_-|-\rangle$, the Schrödinger equation $i|\dot\psi(t)\rangle = H|\psi(t)\rangle$ then implies

$$i\dot{c}_+ = \frac{\omega}{2}(1 + b(t))c_+(t)$$

with a solution

$$c_+(t) = e^{-i\frac{\omega}{2}t}e^{-i\frac{\omega}{2}\int_0^t b(s)\mathrm{d}s}c_+(0).$$

We obtained a solution $|\psi(t)\rangle$ of the Schrödinger equation and now we aim to study its statistics. The basic quantity of interest is an average state, $\mathbb{E}[|\psi(t)\rangle\langle\psi(t)|]$. Note that we are averaging the state not the wave function. The average wave function have no physical meaning because the statistics of measurement outcomes is not linear in the wave function, i.e. for an observable X

$$\mathbb{E}[\mathrm{tr}(\rho X)] = \mathrm{tr}(\mathbb{E}X), \quad \text{but} \quad \mathbb{E}[\langle\psi|X|\psi\rangle] \neq \mathbb{E}[\langle\psi|]X\mathbb{E}[|\psi\rangle],$$

in particular $\mathbb{E}[|\psi\rangle]$ is not even normalized.

The wave function $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ can be written in the basis $|\pm\rangle$ as

$$\rho(t) = \begin{pmatrix} \rho_+ & \rho_{+-} \\ \rho_{+-}^* & \rho_- \end{pmatrix}.$$

Because of the special form of our Hamiltonian the diagonal elements are constant and in particular deterministic. For the off-diagonal elements we have

$$\mathbb{E}[\rho_{+-}(t)] = e^{-i\omega t}\mathbb{E}[e^{-i\omega \int_0^t b(s)\mathrm{d}s}]\rho_{+-}(0).$$

---

[2]From a fundamental perspective this represents lack of our knowledge

The integral can be computed if $b(s)$ is a Gaussian random process. Recall that $X_1, X_2, \ldots, X_n$ is jointly Gaussian if and only if (in many textbooks this is actually taken as a definition)

$$\mathbb{E}[\exp\left(i\sum_n X_n\varphi_n\right)] = \exp\left(-\frac{1}{2}\mathbb{E}[(\sum_n X_n\varphi_n)^2]\right).$$

For the average state we write $\mathbb{E}[(\int_0^t b(s)\mathrm{d}s)^2] = \int_{-t}^t (t - |u|)J(u)\mathrm{d}u$ with $J(s - s') = \mathbb{E}[b(s)b(s')]$ and we have

$$\mathbb{E}[\rho_{+-}(t)] = e^{-i\omega t}e^{-\frac{1}{2}\omega^2\int_{-t}^t(t-|u|)J(u)\mathrm{d}u}\rho_{+-}(0).$$

The correlation function J typically has a bell shape centered at zero and decaying at infinity. If τ is the width of the bell then for $t >> \tau$ we have

$$\int_{-t}^t (t - |u|)J(u)\mathrm{d}u \sim t\int_{-\infty}^\infty J(u)\mathrm{d}u$$

and we see that the averaged off-diagonal element decays exponentially.

We do not pursue the theory beyond this example. We only note that in most experiments external random parameters provide the main contribution to decoherence. Many techniques how to fight this decoherence were invented, the most famous being probably spin echo.

8 Non-demolition measurements

In this section we continue study of experiments of Haroche in which he showed full dynamics of the wave function collapsed in a measurement. In order to prove the collapse we will need a relatively involved results from the theory of stochastic processes. We will recall these results in the following section . The reader not interested in proofs can skip the section, the phenomena captured by Haroche can be understood without it.

Martingales

A pedestrian approach to random variables is to consider them as a quantity with some given probability distribution. Two random variables X, Y are then specified by a join probability distribution $p(x, y)$. A probability distribution of X alone is given by $p(x) = \int p(x, y)\mathrm{d}y$. The conditional probability distribution of X given a value of Y is

$$p(x|y) = p(x, y)/p(x).$$

An important notion in the theory of random variables is a conditional expectation of X given Y,

$$\mathbb{E}[X|Y] = \int xp(x|y)\mathrm{d}x.$$

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Note that this is a function of y and it is random since Y is random. This is a classical equivalent of the partial trace (or rather partial trace is a quantum equivalent of conditional expectation) with the most important property that it recovers expectation of observables that depend only on Y,

$$\mathbb{E}[f(Y)\mathbb{E}[X|Y]] = \mathbb{E}[f(Y)X].$$

Example 14 *Let X be a height of a population sample and Y the sex. Then conditional expectation $\mathbb{E}[X|Y]$ is a random variable with two possible values, average height of men in the sample occurring with a probability that random person in the sample is a man and average height of women in the sample occurring with the probability that random person in the sample is a woman.*

A stochastic process $X_1, X_2, \ldots, X_n$ is a collection of random variables. In the pedestrian way of thinking it is specified by join probability distributions of any finite subset of these variables. A stochastic process is more often specified by a recurrence relation of the form $X_{n+1} = f(X_1, X_2, \ldots X_n)$.

Example 15 *1. The most simple example are identical independent random variables*

$$S_1, S_2, \ldots$$

whose all join probability distribution are products of a single probability distributions, e.g $P(S_1, S_2) = P(S_1)P(S_2)$.

2. A random walk is process defined recurrently by

$$X_{n+1} = X_n + S_n, \quad X_0 = 0$$

where S_n is the process from the previous example. It is called random walk it can be interpreted as tossing a coin S at every step and moving according to the result, X being the position.

Finally a stochastic process is called martingale if

$$\mathbb{E}[X_{n+1}|X_n] = X_n.$$

Martingales play a central role in many areas of probability. A basic result is the Doob's martingale convergence theorem.

Theorem 16 *Suppose that X_n is a bounded martingale then $X_n \to X_\infty$ with a probability 1.*

Example 17 *The notion of martingale (as well as the name) originated from the study of gambling. Let X_n denotes the player capital after nth-round of some gambling game. The capital is a stochastic process with a recurrence relation*

$$X_{n+1} = X_n + f_n(X_n)S_n,$$

where $f_n(X_n)$ represents the quantity the player decided to bet and S_n are independent random variables representing the outcome of the game. The function f_n represents players strategy, how much she is betting depending on time and his current credit. If the player cannot borrow money then $0 \leq f(x) \leq x$. On the other hand we can assume that the function is compactly supported, meaning that the player quits the game if she wins certain amount of money.

This process is a martingale $\mathbb{E}[X_{n+1}|X_n] = X_n$ and the martingale convergence theorem tells us that whatever the betting strategy either the player bankrupts or quits the game with the desired amount of money. A claim not hard to believe.

Non-demolition measurements

The standard projective measurement of a system S in a state $|\psi\rangle$ with respect to a basis $\{|1\rangle, |2\rangle, \dots\}$ reports outcome j with a probability $p_j = |\langle j|\psi\rangle|^2$ and evolves the system into the posterior state $|j\rangle$ upon such event. We aim to see detail dynamics of the transformation (collapse) of the wave function $|\psi\rangle$ into $|j\rangle$. To this end we let the system interact with a series of probes, which are subsequently measured. This picture does not solve the philosophical problem of collapse of the wave function – we still do projective measurements on probes – but it illuminates the process of an interaction of the system with a measurement device.

The theory to be described was motivated by experiments of Haroche. It was derived by Bernard and Breuer [3], I closely follow their article which you may read instead of this section as it is well written and covers the material in the more or less same extent.

For concreteness the probes will be two level systems measured in a $|\pm\rangle$ basis.

Interaction with a single probe

The probe is prepared in a pure state $|G\rangle$ uncorrelated with the system. The interaction of the probe with the system is represented by a unitary U. The join initial state $|\psi\rangle \otimes |G\rangle$ is transformed by the interaction according to

$$|\psi\rangle \otimes |G\rangle \quad \rightarrow \quad U(|\psi\rangle \otimes |G\rangle).$$

Non-demolition measurement (interaction) corresponds to a special choice of U for which the basis vectors $|j\rangle$ are not altered by the evolution. The evolution still acts non-trivially on the probe, $|j\rangle \otimes |G\rangle \rightarrow |j\rangle \otimes U_j|G\rangle$ for some unitary U_j. By linearity this defines the transformation for all initial states,

$$\sum_j \sqrt{p_j}|j\rangle \otimes G \quad \rightarrow \quad \sum_j \sqrt{p_j}|j\rangle \otimes U_j|G\rangle.$$

The probability of measuring $+$ or $-$ on the probe after the interaction is

$$p(\pm) = \sum_j p_j|\langle\pm|U_j|G\rangle|^2$$

and upon measurement result $+$ respectively $-$ the state is transformed into

$$\sum_j \frac{\sqrt{p_j}\langle\pm|U_j|G\rangle}{\sqrt{p(\pm)}}|j\rangle\otimes|\pm\rangle. \tag{12}$$

In particular the population of the *jth*-level in the posterior state given measurement result $\pm$ is

$$\frac{p_j|\langle\pm|U_j|G\rangle|^2}{p(\pm)}. \tag{13}$$

Remark 18 *If we do not measure the probe or discard the measurement result, the transformation acts on the system as a certain Kraus map $\mathcal{K}$. From the Eq. (12) we can read how this map acts, $\mathcal{K}(|j\rangle\langle k|) = \langle G|U_k^*U_j|G\rangle|j\rangle\langle k|$. This is a dephasing map and if the non-degeneracy condition $|\langle G|U_k^*U_j|G\rangle| \neq 1$ is satisfied the states $|j\rangle$ and $|k\rangle$ are distinguishable.*

Sequence of probes

We consider a sequence of probes successively interact with the system. Although it is not essential when we measure the probes, it is easier to think that n-th probe was measured before the $n+1$-th probe begin to interact with the system.

Let $p_j^{(n)}$ be the population of j-th level of the system after measurement of the n-th probe. $p_j^{(n))}$ depends on the sequence of measurement results, e.g. $+ - - + \ldots$, on preceding probes. These measurement results are random and $p_j^{(n)}$ is a stochastic process with recurrence relation given by Eq. (13),

$$p_j^{(n+1)} = \begin{cases} \frac{p_j^{(n)}|\langle+|U_j|G\rangle|^2}{p^{(n)}(+)} & \text{with prob.} \quad p^{(n)}(+) \\ \frac{p_j^{(n)}|\langle-|U_j|G\rangle|^2}{p^{(n)}(-)} & \text{with prob.} \quad p^{(n)}(-), \end{cases}$$

where $p^{(n)}(\pm)$ is a probability to measure outcome $\pm$ on the n-th probe given populations $p_j^({}n)$, i.e.

$$p^{(n)}(\pm) = \sum_j p_j^{(n)}|\langle\pm|U_j|G\rangle|^2.$$

The following theorem describes the behavior of this stochastic process and connects non-demolition measurement with the standard projection measurement. To easy the comparison, recall that such a measurement transforms the state into $|j\rangle$ with a probability $p_j^{(0)}$.

Theorem 19 *Stochastic process of populations $p_j^{(n)}$ has a limit p_j^∞.*
Suppose furthermore that the measurement satisfies a non-degeneracy condition

$$|\langle+|U_j|G\rangle|^2 \neq |\langle+|U_k|G\rangle|^2 \quad \text{for all} \quad k \neq j,$$

then p_j^∞ is either zero or one with a probability of a corresponding projection measurement.

$$p_j^\infty = \begin{cases} 1 & \text{with prob.} \quad p_j^{(0)} \\ \\ 0 & \text{with prob.} \quad p_j^{(0)}. \end{cases}$$

Proof: The key observation is that the stochastic process $p_j^{(n)}$ is a martingale. The first statement, on the existence of limiting populations, then follows from Doob's convergence theorem. That $p_j^{(n)}$ is martingale is a simple computation,

$$\mathbb{E}[p_j^{(n+1)}|p_j^{(n)}] = \frac{p_j^{(n)}|\langle+|U_j|G\rangle|^2}{p^{(n)}(+)}p^{(n)}(+) + \frac{p_j^{(n)}|\langle-|U_j|G\rangle|^2}{p^{(n)}(-)}p^{(n)}(-)$$
$$= p_j^{(n)}(|\langle+|U_j|G\rangle|^2 + |\langle-|U_j|G\rangle|^2) = p_j^{(n)}.$$

We now assume the non-degeneracy condition and we want to prove the zero-one law for the limiting distribution of populations. Suppose for contradiction that p_j^∞ and p_k^∞ are non-zero for $j \neq k$. The non-degeneracy condition implies that $|\langle+|U_j|G\rangle|^2$ and $|\langle+|U_k|G\rangle|^2$ cannot be simultaneously zero and in particular the limit probability to measure $+$, $p^\infty(+) = \sum_j p_j^\infty|\langle+|U_j|G\rangle|^2$, is positive. The limiting probability will not change upon measuring $+$,

$$p_j^\infty = \frac{p_j^\infty|\langle+|U_j|G\rangle|^2}{p^\infty(+)}, \quad p_k^\infty = \frac{p_k^\infty|\langle+|U_k|G\rangle|^2}{p^\infty(+)}.$$

It follows form the equations that $|\langle+|U_j|G\rangle|^2 = |\langle+|U_k|G\rangle|^2$, which is a contradiction.

If p_j^∞ is not zero for only one level then it has to be equal to 1 due to the conservation of probability.

Since the process is a martingale, $\mathbb{E}[p_j^{(n)}] = p_j^{(0)}$. In particular

$$p_j^{(0)} = \mathbb{E}[p_j^\infty] = Prob(p_j^\infty = 0)0 + Prob(p_j^\infty = 1)1,$$

which proves the final claim. □.

Remark 20   *1. You might have noticed that the non-degeneracy condition for the Kraus map (see Remark 18) and the non-degeneracy condition of the Theorem are different. The reason is that even though the interaction might distinguish between j and k the measurement with respect to some basis might not. However if the Kraus map is not degenerate you can always find a "good" measurement that will distinguish the states. Formally, if $|\langle G|U_k^*U_j|G\rangle| \neq 1$ then there exist a basis $|\pm\rangle$ on the probe such that $|\langle+|U_j|G\rangle|^2 \neq |\langle+|U_k|G\rangle|^2$.*

    2. In wider perspective the theorem belongs to a family of zero-one laws describing (in various settings) the emergence of a fact. The statement "quantum state is in the level j" becomes asymptotically true or false with certain probability, a fact emerged.

The last question I want to address is how do you distinguish which level becomes asymptotically occupied from the sequence of measurement results. This is a random sequence and the information is encoded in the frequencies of $\pm$. In particular given that only level j is populated, i.e. $p_j = 1$, we have $p(+) = |\langle +|U_j|G\rangle|^2$. Given the non-degeneracy condition this means that a sign of approaching level j is that frequencies of $+$ results approach $|\langle +|U_j|G\rangle|^2$.

If you are not familiar with stochastic processes it might be hard for you to imagine how all this works, how random sequence of pluses and minuses changes occupation levels, how they approach some (random) final outcome, etc. If that is the case and you want to invest energy into understanding the topic, I suggest that you write a small computer program to simulate the stochastic process, for some chosen $|G\rangle$ and U_j and $|\pm\rangle$.

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