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Introduction to theory of open quantum systems

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Literature

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[2] H.-P. Breuer i F. Petruccione, The Theory of Open Quantum Systems, New York: Oxford University Press, 2002.

[3] Á. Rivas i S. F. Huelga, Open Quantum Systems, Berlin Heidelberg: Springer, 2012.

[4] C. Chicone, Ordinary Differential Equations with Applications, New York: Springer, 2006.

1. Mathematical elements

For a convenience of the Reader, we begin our series of lectures with a not-so-long, yet quite comprehensive mathematical introduction, which will provide a kind of a toolbox, necessary for proper understanding of the whole material. The first part of this introduction will be a simple reminder of some basic, but powerful, algebraic structures broadly used in theoretical physics. Next, we will introduce some basic elements of theory of ordinary differential equations in vector spaces and finally, we will introduce some basic examples of matrix norms.

1.1. Basic algebraic structures

We start with some really basic, fundamental concepts, which the reader should be already quite familiar with. Those will include a *semigroup*, *group*, *field*, *vector space* and then *algebra*.

1.1.1. Semigroups and groups

Definition 1. (Semigroup) Let G be a non-empty set. An order pair $(G,\circ)$, where $\circ$ is a binary operation on G, is called a *semigroup* if and only if the operation $\circ$ is *associative*, which means, that

$$\forall\, a,b,c \in G : (a \circ b) \circ c = a \circ (b \circ c).$$

If, in addition, there exists some element $e \in G$ which is a *neutral element* of operation $\circ$, namely if it satisfies property

$$\forall\, a \in G : a \circ e = e \circ a = a,$$

such semigroup $(G,\circ)$ is called a **monoid** in literature. From now on, however, we will be interested only in semigroups with neutral elements, and we will be simply referring to them as "semigroups". The notion of a semigroup will be of particular importance for us later on.

Definition 2. (Group) Let $(G,\circ)$ be a semigroup. If every element of G is *invertible* with respect to operation $\circ$, namely if the following property holds

$$\forall\, a \in G\ \exists\, a^{-1} \in G : a \circ a^{-1} = a^{-1} \circ a = e,$$

then such semigroup $(G,\circ)$ is called a *group*. Moreover, if operation $\circ$ is *commutative*, i.e. if it satisfies property

$$\forall\, a,b \in G : a \circ b = b \circ a,$$

group $(G,\circ)$ is called a *commutative group* or *abelian group*.

Examples of semigroups and groups

It turns out, that groups and semigroups are very common structures, broadly appearing in whole mathematics. Below we give few basic examples. The reader is encouraged to check, if they really satisfy all the axioms given in respective definitions:

a) Structure $(\mathbb{Z}_0,+)$, where $\mathbb{Z}_0$ stands for a set of non-negative integers (i.e. $\mathbb{Z}_0 = \{0,1,2,\dots\}$) and $+$ is the "usual" addition, is a semigroup (a monoid, to be precise). Number 0 is then a neutral element.

b) Structure $(\mathcal{C}([0,1]),\circ)$, where $\mathcal{C}([0,1])$ is a set of all real, continuous functions defined on interval $[0,1]$ and $\circ$ stands for composition of functions (such that $(f \circ g)(x) = f\big(g(x)\big)$), is a semigroup (again – a monoid) with identity function serving as a neutral element.

c) Structures $(\mathbb{Z},+)$, $(\mathbb{R},+)$, $(\mathbb{C},+)$ with $\mathbb{Z}$, $\mathbb{R}$ and $\mathbb{C}$ being sets of integers, reals and complex numbers, respectively and $+$ being a "usual" addition in appropriate set, are groups.

d) Structure $\left(M_d^{\text{inv.}},\cdot\right)$, where $M_d^{\text{inv.}}$ Is a set of all *invertible* square matrices of size d and $\cdot$ is a matrix multiplication, is a group.

e) Let A be a fixed, square matrix of size d. Then, a structure $(\{e^{tA} : t \geq 0\},\cdot)$, where e^{tA} is an exponential of matrix tA and $\cdot$ is a usual matrix multiplication, forms a semigroup (monoid, actually). This example will be of particular importance for us in Section 1.3 and Section 7, where we will introduced the Holy Grail of open quantum systems theory, namely the Quantum Dynamical Semigroup.

1.1.2. Algebraic fields

Definition 3. An algebraic structure $(K,+,\circ)$, where K is non-empty and $+$, $\circ$ are two associative and commutative binary operations on K, called the „addition" and „multiplication", respectively, will be called a *field*, when there exist two special elements in K, denoted 1 and 0, such that

1. structure $(K,+)$ is an abelian group with 0 serving as a neutral element of addition,
2. structure $(K \setminus \{0\},\circ)$ is an abelian group with 1 serving as a neutral element of multiplication, and
3. multiplication distributes over addition, i.e. it holds, that

$$\forall\, a,b,c \in K : a \circ (b+c) = a \circ b + a \circ c.$$

The theory of fields is one of the most prominent and fruitful domains in abstract algebra, very deep and well-studied. The general motivation standing behind introduction of fields is the necessity of defining structures equipped with four basic operations, like addition, subtraction, multiplication and division, which behave like and posses properties similar to the "usual", corresponding operations on real numbers. Basic, archetypic examples of fields are $(\mathbb{R},+,\cdot)$ and $(\mathbb{C},+,\cdot)$, where $+$ and $\cdot$ are the "usual" operations of addition and multiplication in sets $\mathbb{R}$ or $\mathbb{C}$. Another, maybe more nonobvious example is $(\mathbb{Q},+,\cdot)$ where $\mathbb{Q}$ is a set of rational numbers and the addition and multiplication operations are defined just like those on real numbers (this field is actually the subfield of reals).

1.1.3. Vector spaces and algebras

In this section we briefly sketch the theory of linear spaces and closely related algebras. The importance of both linear space and algebra for pure mathematics and all related areas of study is immense. One could probably safely say that the concept of linear space, and all the other resulting constructs, as metric, Banach and Hilbert spaces, have shaped theoretical physics into a form which it exhibits now. The Banach and Hilbert space concept should be already familiar for the Reader; we will, however, still provide a fundamental background in the succeeding subsection. We start with a very general, broad notion of a vector space:

Definition 4. (Vector space) Let $\mathbb{K} = (K,+,\cdot)$ be a field and let V be a nonempty set. An algebraic structure $(V,\mathbb{K},\oplus,\circ)$ such that $(V,\oplus)$ is an abelian group and $\circ$ is an operation $\mathbb{K} \times V \mapsto V$ which satisfies all the following axioms,

1. $\forall\, a \in \mathbb{K}\, \forall\, x,y \in V : a \circ (x \oplus y) = a \circ x \oplus a \circ y$,
2. $\forall\, a,b \in \mathbb{K}\, \forall\, x \in V : (a+b) \circ x = a \circ x \oplus b \circ x$,
3. $\forall\, a,b \in \mathbb{K}\, \forall\, x \in V : a \circ (b \circ x) = (a \cdot b) \circ x$, and
4. $\forall\, x \in V : 1_{\mathbb{K}} \circ x = x$ for $1_{\mathbb{K}}$ being the neutral element of multiplication in $\mathbb{K}$,

is called a *linear space* or *vector space over field* $\mathbb{K}$.

Rephrasing the above definition into a non-formal semantics one could say, roughly, that "vector space may be understood as a set of elements (called simply vectors) which can be scaled (by means of multiplying them by scalars from $\mathbb{K}$) and added together, producing some other vector inside this set". Since the notion of vector space is so basic and fundamental, we assume that the Reader is already familiar with it and so we will not be giving examples of vector spaces here, but in the next section instead, which will deal with more specialized vector spaces equipped with additional, topological structure, such as Hilbert spaces.

From now on, we will be simplifying our notation in such a way, that certain, natural operations on vector spaces, such as vector addition and multiplication of vectors and numbers will be denoted in the most natural way with possibly simplest symbols, i.e. instead of typing $x \oplus y$ for vector addition we simply write $x + y$, and instead of $a \circ x$ we put ax, or $a \cdot x$. The Reader should notice that the exact meaning of symbols used for denoting vector-valued operations will be immediately clear from the context and should not lead to any confusion.

Definition 5. (Algebra and *-algebra) Let V be a vector space over field $\mathbb{K}$ and let $\cdot$ be a binary operation on V. If for all vectors $x, y, z \in V$ and all $\alpha, \beta \in \mathbb{K}$ the following conditions hold,

1. $(x + y) \cdot z = x \cdot z + y \cdot z$ (right distributivity of multiplication over addition),
2. $x \cdot (y + z) = x \cdot y + x \cdot z$ (left distributivity of multiplication over addition),
3. $(\alpha x) \cdot (\beta y) = (\alpha\beta)(x \cdot y)$ (compatibility with multiplication of scalars),

then the algebraic structure $\mathcal{A} = (V, \cdot)$ is called the *algebra over field* $\mathbb{K}$.

If, in addition, there exists an element $I \in V$ which is a neutral element for operation $\cdot$, then $\mathcal{A}$ is sometimes called a *unital algebra* or an *algebra with identity*. If the operation $\cdot$ is associative then $\mathcal{A}$ is called an *associative algebra*, and if it is commutative – an *abelian algebra* or *commutative algebra*.

Amongst all the algebras, a special attention is granted to the case of so-called **-algebras*. Namely, one introduces yet another operation on V, called the *involution*, which we will be denoting with a $*$ symbol. It is required to satisfy the following axioms for all $x, y \in V$ and $\alpha, \beta \in \mathbb{K}$:

1. $(\alpha x + \beta y)^* = \bar{\alpha} x^* + \bar{\beta} y^*$ (conjugate-linearity),
2. $(xy)^* = y^* x^*$,
3. $x^{**} = (x^*)^* = x$ (involutiveness),
4. $1^* = 1$, where 1 is the neutral element in $\mathcal{A}$ (if exists).

If such operation exists, structure $(V, \cdot, *)$ is called **-algebra over field* $\mathbb{K}$.

1.2. Hilbert spaces

In this subsection we will briefly recollect some basic facts and properties of Hilbert spaces, which is by far the most prominent mathematical construction to have an impact within theoretical physics. The Reader most probably already realises, that significance of notion of a Hilbert space is so great, that in fact one could describe the entire quantum mechanics as a subset of a theory of bounded and unbounded linear operators acting on in general infinite-dimensional Hilbert spaces.

1.2.1. Norm and inner product

One on the most natural structure, which we can demand from vector space is the notion of a length of a vector. In mathematical language, such length is defined – in more generalized manner – as a certain, nonnegative function defined on a vector space which assigns to vector $x \in V$ some number $\|x\| \geq 0$, called the **norm** of x. We have the following definition:

Definition 6. (Norm) Let V be a vector space over field $\mathbb{K}$. A function $\|\cdot\| : V \to [0,\infty)$ satisfying, for all $x, y \in V$ and all $a \in \mathbb{K}$, conditions

1. $\|ax\| = |a| \cdot \|x\|$,
2. $\|x + y\| \leq \|x\| + \|y\|$,
3. $\|x\| = 0 \Leftrightarrow x = 0$,

is called the *norm* on space V. Space V equipped with a norm is called the *normed space*.

Recall, that one can introduce in a vector space V yet another, specialized two-argument function, here denoted by angle brackets as $\langle\cdot,\cdot\rangle$, mapping pairs of vectors into scalars, called the **inner product** on V. The formal definition of an inner product is the following:

Definition 7. (Inner product) Let V be a vector space over field $\mathbb{K}$. A two-argument, $\mathbb{K}$-valued function $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{K}$ is called the *inner product* on V if and only if it satisfies the following conditions for all vectors $x, y, z \in V$ and all scalars $a, b \in \mathbb{K}$:

1. $\langle x, x\rangle \geq 0$ and $\langle x, x\rangle = 0$ if and only if $x = 0$,
2. $\overline{\langle x, y\rangle} = \langle y, x\rangle$ (conjugate symmetry),
3. $\langle x, ay + bz\rangle = a\langle x, y\rangle + b\langle x, z\rangle$ and $\langle ax + by, z\rangle = \bar{a}\langle x, z\rangle + \bar{b}\langle y, z\rangle$ (sesquilinearity).

Vector space V equipped with some inner product is then often called *the inner product space*.

By introducing the inner product on some vector space, we are given a powerful tool for analysis of V itself together with its linear subspaces, as well as many properties of functions defined on, or with values in V. For example, with inner product we are now able to define very intuitive notions, such as orthogonality relations between vectors and subspaces, length of a vector and angle between two vectors. To be more precise, the length of a vector may be always introduced by applying inner product on V in such a way, that one defines norm $\|x\|$ of any vector $x \in V$ in such a way, that

$$\|x\| = \sqrt{\langle x, x\rangle}.$$

In a result, any inner product space automatically also becomes a normed space and the norm given by the above prescription is often called *generated* or *induced by inner product*. The Reader is encouraged to check that the above formula indeed gives a well-defined norm on V.

1.2.2. Hilbert space

In order to introduce the notion of Hilbert space, which is by far probably the most important and prominent mathematical construct ever to find application in quantum theory, we must remind ourselves the concept of *completeness* of vector spaces. Shortly, a normed space will be called *complete* if and only if it assures convergence of well-behaved sequences inside itself.

Let then (x_n) be some sequence of vectors in a normed vector space $(V, \|\cdot\|)$. Such sequence is called a **Cauchy sequence** if and only if distances between its subsequent elements become smaller and smaller, or, more formally, if

$$\forall\, \epsilon > 0\ \exists\, N > 0\ \forall\, n, m > N : \|x_n - x_m\| < \epsilon,$$

which can be equivalently put as a simple, computationally friendly condition

$$\lim_{n,m\to\infty} \|x_n - x_m\| = 0.$$

The Reader may recall that in case of real-valued sequences, or – more broadly – in any finite-dimensional, real Euclidean space a sequence was convergent if and only if it was Cauchy. It turns out,

that **in general case of infinite-dimensional normed spaces it does not have to be so**. Namely, it may happen, that in certain normed spaces, Cauchy sequences will not be convergent, i.e. their "limits" will not exist inside this space or will be simply divergent[1]. Those normed spaces, which are "well-behaved" in this manner, will be then called **complete** and are of special importance for both functional analysis and physics:

Definition 8. (Complete space) Let $(V, \|\cdot\|)$ be a normed vector space. If every Cauchy sequence (x_n) of elements of V converges to some element $x \in V$, then space V is called *complete*[2] *vector space*, or *Banach space*.

Now we are eventually ready to introduce a celebrated notion of Hilbert space, by combining somewhat disjoint notions of inner product and completeness, into one elegant construct:

Definition 9. (Hilbert space) An inner product space H is called the *Hilbert space*, if it is complete with respect to the norm induced by inner product.

By their nature, one may also characterize Hilbert spaces as a (possibly) infinite-dimensional counterparts of finite-dimensional Euclidean spaces, which resemble their properties in possibly best achievable way and therefore are particularly convenient to work with.

1.3. Ordinary differential equations in vector spaces

In this section we present an overview of theory of ordinary differential equations (ODEs) in vector spaces, which will become a necessity for introducing the concept of Master Equation describing quantum evolution later on. For the sake of clarity, we will restrict ourselves solely to the case of vector spaces with finite dimension and only to first-order ODEs.

1.3.1. Preface: vectors and operators in finite-dimensional spaces

Let $(V, \|\cdot\|)$ be a normed vector space of finite dimension d (for now, we make no restrictions for choice of a norm) over field $\mathbb{C}$ of complex numbers, so space V may be canonically isomorphic to space $\mathbb{C}^d$ of complex sequences of length d. Such isomorphism is then introduced by defining a **basis** in V. Namely, denote by $\{e_i\}$ a family of linearly independent vectors, *spanning* V. This means, that there exists exactly d vectors $e_1, e_2, \dots, e_d \in V$, such that family $\{e_i\}$ is linearly independent[3] and every vector $x \in V$ may be represented as a linear combination

$$x = \sum_{i=1}^{d} x_i e_i = x_1 e_1 + x_2 e_2 + \cdots + x_d e_d$$

for some **unique** sequence of coefficients $(x_1, x_2, \dots x_d) \in \mathbb{C}^d$. One can easily show that every vector $x \in V$ is indeed uniquely represented by a sequence (x_i) and vice versa, by showing that the mapping $x \mapsto (x_i)$ is a **bijection**, and therefore spaces V and $\mathbb{C}^d$ are isomorphic. From now on, we will be freely making use of this isomorphism $V \simeq \mathbb{C}^d$, referring to *vectors* or *sequences* interchangeably. Moreover, the common approach allows to reinterpret vector x as a *one-column matrix* populated with its coefficients x_i, so in particular we have three equivalent ways of expressing vectors in finite-dimensional spaces:

[1] Remember, that although Cauchy sequence may not be convergent at all, a reverse statement always holds, namely every convergent sequence is automatically a Cauchy sequence.
[2] In general, *completeness* refers to much broader class of *metric spaces*, which may not be vector spaces at all.
[3] Recall, that family of vectors $\{e_i : 1 \leq i \leq d\}$ is called *linearly independent* if $a_1 e_1 + a_2 e_2 + \cdots + a_d e_d = 0$ implies $a_1 = a_2 = \cdots = a_d = 0$. Equivalently, one can say that $\{e_i\}$ is linearly independent if and only if no vector e_i may be expressed as a linear combination of vectors of this family, other than e_i.

$$x = \sum_{i=1}^{d} x_i e_i \quad \leftrightarrow \quad (x_i) = (x_1, \dots, x_d) \quad \leftrightarrow \quad \hat{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix}.$$

Now, let $T : V \to V$ to be any **linear operator** acting on V. By utilizing our isomorphism $V \simeq \mathbb{C}^d$ we see, that while each vector $x \in V$ is represented as a sequence of its components in some preselected basis $\hat{x} = (x_i)$ or as a column vector populated with its components, also operator T is then representable as a *square matrix* $\hat{T} = [t_{ij}]$ of size d. In such case, action of map T on vector x, i.e. element $T(x)$, may be uniquely represented as a multiplication of matrices $\hat{T}\hat{x}$:

$$T(x) \quad \leftrightarrow \quad \hat{T}\hat{x} = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{d1} \\ t_{21} & t_{22} & \cdots & t_{d2} \\ \vdots & \vdots & \ddots & \vdots \\ t_{d1} & t_{d2} & \cdots & t_{dd} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix}.$$

1.3.2. Derivatives and ODEs in vector spaces

We are now ready to introduce some basic theory of ordinary differential equations in spaces of finite dimension and characterize their solutions.

Let $\mathcal{I} \subseteq \mathbb{R}$ be some open interval on the real line. Consider a *vector-valued function* $t \mapsto x_t \in V$, where $t \in \mathcal{I}$ and

$$x_t = \sum_{i=1}^{d} x_i(t) e_i$$

for some complex-valued functions $x_1, x_2, \dots, x_d : \mathcal{I} \to \mathbb{C}$, all defined on interval $\mathcal{I}$.

Definition 10. (Derivative of vector-valued function) We say that a function $t \mapsto x_t$ is *differentiable*[4] *in interval* $\mathcal{I}$ if and only if there exists a function $t \mapsto x'_t$ such that for each $t \in \mathcal{I}$ we have

$$\lim_{h \to 0} \left\| \frac{x_{t+h} - x_t}{h} - x'_t \right\| = 0.$$

Then, function x'_t is simply called *the derivative* of x_t. Symbolically, we have

$$x'_t = \frac{dx_t}{dt} = \lim_{h \to 0} \frac{x_{t+h} - x_t}{h}.$$

The class of differential equations, which we will be interested in, will be given as the ODE of a form

$$\frac{dx_t}{dt} = A_t(x_t),$$

where x_t is some **unknown function** and operator $A_t : V \to V$ is of a **known form** and may also be dependent on the variable t. If indeed A_t is some explicit function of t, the ODE will be called *nonautonomous*. If, on the other hand, $A_t = A$ is some constant operator, the ODE is called *autonomous*. Unfortunately, nonautonomous ODEs are in general very tough to solve analytically and there exists no general schemes for obtaining solutions of such equations, apart from some very general and abstract formal expressions (such as time-ordered exponentials or Dyson series) and we will not be exploring these. Instead, we will focus on much more convenient and computationally accessible case of autonomous equations.

[4] Differentiability in this sense is a simple generalization of *pointwise differentiability*.

We stress here, that differentiability of vector-valued functions in finite dimensional case is completely equivalent to differentiability of all functions $x_i(t)$, i.e. a vector-valued function $t \mapsto x_t$ is differentiable if and only if it is given by differentiable coefficients:

Theorem 1. Let $(V, \|\cdot\|)$ be a finite dimensional normed vector space and let $t \mapsto x_t$, $t \in \mathcal{I}$, be a vector valued function on V such that $x_t = \sum_{i=1}^{d} x_i(t) e_i$. Then, function x_t is differentiable if and only if all functions $x_i(t)$ are differentiable in $\mathcal{I}$. In such scenario, one simply has

$$\frac{dx_t}{dt} = \sum_{i=1}^{d} \frac{dx_i(t)}{dt} e_i.$$

We leave the proof to the Reader.

1.3.3. Solutions and state transition matrices

From now on, we will be heavily utilizing the isomorphism between V and $\mathbb{C}^d$ in such a way, that we will be explicitly rephrasing all vector quantities and linear operators in terms of their respective matrix representations and we will be ignoring distinction, say, between objects x and $\hat{x}$ and A and $\hat{A}$, abusing the notation a little bit. Basing on Section 1.3.1 we see, that we can rewrite the general, nonautonomous equation $\frac{dx_t}{dt} = A_t(x_t)$ into equivalent, *matrix* form

$$\frac{dx_t}{dt} = A_t x_t.$$

Now, we introduce the so-called fundamental matrix solution of the ODE, however we will not overly formal and precise here; this entire part of the lecture is heavily based on a book by C. Chicone [1] and the Reader may find all the underlying mathematical machinery therein.

Theorem 2. There exists a differentiable, matrix-valued function $t \mapsto \Phi_t$, $t \in \mathcal{I}$, such that it is a solution of a corresponding, matrix differential equation

$$\frac{d\Phi_t}{dt} = A_t \Phi_t,$$

and Φ_t is invertible for all $t \in \mathcal{I}$. Such matrix Φ_t is then called the *fundamental matrix solution* of the ODE in question. If, in addition it happens that $\Phi_{t_0} = I$ (the identity matrix) for some $t_0 \in \mathcal{I}$, then Φ_t is called the *principal fundamental matrix solution*.

The strength of a notion of fundamental matrix solution is such, that by acting with this matrix on any fixed vector in V we obtain some solution to the original ODE, just like the following theorem implies:

Theorem 3. Let Φ_t to be a fundamental matrix solution of an ODE of a form $\frac{dx_t}{dt} = A_t x_t$. Then, a vector-valued function of a form

$$x_t = \Phi_t c,$$

where $c \in \mathbb{C}^d$, is a *general solution* of the ODE in question.

Proof. It suffices to differentiate x_t:

$$\frac{dx_t}{dt} = \frac{d}{dt}(\Phi_t c) = \frac{d\Phi_t}{dt} c = A_t \Phi_t c = A_t x_t,$$

so indeed the proposed function x_t satisfies the ODE. □

Note, that by choosing some concrete vector $c \in V$ we obtain a *particular solution* of the ODE: let us assume, that we seek for a solution satisfying a certain initial value problem, i.e. we want the solution x_t to satisfy $x_{t_0} = w$ for some $t_0 \in \mathcal{I}$. From invertibility of Φ_t we immediately notice, that

$$w = x_{t_0} = \Phi_{t_0} c \quad \Rightarrow \quad c = \Phi_{t_0}^{-1} w \quad \Rightarrow \quad x_t = \Phi_t \Phi_{t_0}^{-1} w.$$

However, we easily notice that the new matrix-valued function

$$\Psi_t = \Phi_t \Phi_{t_0}^{-1}$$

also must be invertible and is also a solution to the matrix ODE, since

$$\frac{d}{dt}\Psi_t = \left(\frac{d}{dt}\Phi_t\right)\Phi_{t_0}^{-1} = A_t \Phi_t \Phi_{t_0}^{-1} = A_t \Psi_t$$

and so provides another fundamental matrix solution; however, putting $t = t_0$ we immediately have $\Psi_{t_0} = I$, so such function is the *principal fundamental matrix solution*. In fact, if Φ_t is (any) fundamental matrix solutions, then one can always construct a fundamental matrix solution $\Psi_t = \Phi_t \Phi_{t_0}^{-1}$ for any $t_0 \in \mathcal{I}$ which will be principal. Such a construct allows to define yet another, useful object, the state transition matrix:

Definition 11. (State transition matrix) A two-variable function $(t, s) \mapsto \Psi_{t,s}$ such that, for each $s \in \mathcal{I}$, a one-variable function $t \mapsto \Psi_{t,s}$ is a fundamental matrix solution and $\Psi_{t,t} = I$, is called the *state transition matrix* of the ODE in question.

Theorem 4. Let $t \mapsto \Phi_t$, $t \in \mathcal{I}$, be a fundamental matrix solution. Then, a two-variable matrix function

$$\Psi_{t,s} = \Phi_t \Phi_s^{-1}$$

is the state transition matrix of the ODE in question. Moreover, $\Phi_{t,s}$ satisfies so-called *Chapman-Kolmogorov identities*:

1. $\Psi_{t,t} = I$,
2. $\Psi_{t,s}\Psi_{s,u} = \Psi_{t,u}$,
3. $\Psi_{t,s}^{-1} = \Psi_{s,t}$,
4. $\frac{d}{ds}\Psi_{t,s} = -\Psi_{t,s}A_s$.

Proof. Again, the proof is left for the Reader as an exercise.

1.3.4. Autonomous ODE in vector space

We grant a special attention to the case of autonomous ODE in vector space, namely and ODE of a form

$$\frac{dx_t}{dt} = Ax_t,$$

where again $t \in \mathcal{I}$ for some open interval $\mathcal{I} \subset \mathbb{R}$, where A is some square matrix of dimension d. In such case, one can immediately characterize all solutions of this ODE in terms of the following theorem:

Theorem 5. The fundamental matrix solution of autonomous ODE of a form $\frac{dx_t}{dt} = Ax_t$, $t \in \mathcal{I}$, is expressible in terms of a matrix exponential as

$$\Phi_t = e^{tA}C, \qquad t \in \mathcal{I},$$

where C is some invertible square matrix. Moreover, principal fundamental matrix Ψ_t and state transition matrix $\Psi_{t,s}$ take a simple form

$$\Psi_t = e^{(t-t_0)A}, \qquad \Psi_{t,s} = e^{(t-s)A}.$$

Exponentiation of a square matrix is defined in terms of a formal power series

$$e^T = \sum_{n=0}^{\infty} \frac{T^n}{n!} = I + T + \frac{1}{2}T^2 + \frac{1}{6}T^3 + \cdots$$

which converges absolutely in $M_d(\mathbb{C})$, such that we have

$$e^{tA} = I + tA + \frac{t^2A^2}{2} + \frac{t^3A^3}{6} + \cdots = \sum_{n=0}^{\infty} \frac{t^n}{n!}A^n.$$

Proof. Left as an exercise.

Diagonalizable case

For simplicity, let us assume for a moment that matrix A is *diagonalizable*, i.e. that it is similar to a diagonal matrix, namely, that there exists some invertible matrix P and a diagonal matrix D, that

$$A = PDP^{-1}.$$

One can show, that matrix A is diagonalizable if and only if the sum of dimensions of its eigenspaces is equal to dimension of the whole vector space V (d in our case), or, that it has exactly $\dim V$ linearly independent eigenvectors v_i, which then form a basis of V (not necessarily orthogonal!). This means, that the eigenequation of matrix A,

$$Av_i = \lambda_i v_i, \qquad i = 1, \ldots, d$$

is satisfied for exactly d eigenvectors v_i and some eigenvalues $\lambda_i \in \mathbb{C}$. Recall, that a number λ_i is the eigenvalue of A if and only if it is a root of a characteristic polynomial[5] of A, i.e. if it satisfies

$$\det(A - \lambda_i I) = 0.$$

One can check that matrix P represents a transformation to a coordinate frame given by eigenvectors matrix A and may be built from the eigenvectors of A stacked as columns, one by one, and matrix D is diagonal and populated with eigenvalues of A, i.e.

$$P = \left(\begin{bmatrix} \\ v_1 \\ \\ \end{bmatrix}, \begin{bmatrix} \\ v_2 \\ \\ \end{bmatrix}, \ldots, \begin{bmatrix} \\ v_d \\ \\ \end{bmatrix}\right), \qquad D = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_d \end{pmatrix}.$$

If this is the case, one can check, that the fundamental matrix solution Φ_t of our ODE has particularly simple form

$$\Phi_t = e^{tA}P = \left(e^{t\lambda_1}\begin{bmatrix} \\ v_1 \\ \\ \end{bmatrix}, e^{t\lambda_2}\begin{bmatrix} \\ v_2 \\ \\ \end{bmatrix}, \ldots, e^{t\lambda_d}\begin{bmatrix} \\ v_d \\ \\ \end{bmatrix}\right),$$

and principal fundamental and state transition matrices are just like earlier,

$$\Psi_t = e^{(t-t_0)A}, \qquad \Psi_{t,s} = e^{(t-s)A}.$$

We recall here, that if matrix A is diagonalizable, i.e. $A = PDP^{-1}$, then its exponential admits particularly simple form

[5] Keep in mind, that number of roots of characteristic polynomial depends on the field used. It may happen, that a matrix is not diagonalizable over field $\mathbb{R}$, but may be diagonalizable over field $\mathbb{C}$, which is algebraically closed. In this situation, any (real or complex) square matrix of size d has exactly d complex eigenvalues.

$$e^A = e^{PDP^{-1}} = Pe^D P^{-1} = P\begin{pmatrix} e^{\lambda_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{\lambda_d} \end{pmatrix} P^{-1}.$$

Example 1. Assume we have a following autonomous ODE in space $V \simeq \mathbb{C}^2$:

$$\frac{d}{dt}\begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}.$$

We will find its principal fundamental matrix solution. First, we check, that the matrix A is a normal matrix,

$$\begin{aligned} AA^* - A^*A &= \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix} - \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}\begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix} \\ &= \begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} - \begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} = 0, \end{aligned}$$

so from general linear algebra we know that it is diagonalizable. Next, we find its eigenvalues by solving the characteristic polynomial $\det(A - \lambda I) = 0$ for λ:

$$\det(A - \lambda I) = \det\begin{pmatrix} 2-\lambda & -1 \\ 1 & 2-\lambda \end{pmatrix} = (2-\lambda)^2 + 1 = 0,$$

which has solutions $\lambda_1 = 2 + i$, $\lambda_2 = 2 - i$, which yield

$$D = \begin{pmatrix} 2+i & 0 \\ 0 & 2-i \end{pmatrix}.$$

The Reader is then encouraged to check, that the (normalized) eigenvectors v_1, v_2 are of a form

$$v_1 = \begin{pmatrix} \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad v_2 = \begin{pmatrix} \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

and so, the diagonalizing matrix P is of a form

$$P = \left(\begin{bmatrix} v_1 \end{bmatrix}, \begin{bmatrix} v_2 \end{bmatrix}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix}.$$

We observe that vectors v_1 and v_2 are mutually orthogonal in $\mathbb{C}^2$,

$$\langle v_1, v_2 \rangle = \frac{1}{2}(-i \quad 1)\begin{pmatrix} -i \\ 1 \end{pmatrix} = \frac{1}{2}(i^2 + 1) = 0,$$

which yields, that matrix P is unitary. Indeed, we check, that

$$PP^* = \frac{1}{\sqrt{2}}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix}^* = \frac{1}{2}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix}\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

so we have $PP^* = I$ and so $P^{-1} = P^*$,

$$P^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}.$$

We can also confirm that matrix A is then diagonalized by P,

$$P^{-1}AP = \frac{1}{\sqrt{2}}\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}\begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2+i & 0 \\ 0 & 2-i \end{pmatrix} = D,$$

as it should be. This allows to compute e^{tA},

$$e^{tA} = Pe^{tD}P^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix}\begin{pmatrix} e^{(2+i)t} & 0 \\ 0 & e^{(2-i)t} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}$$

$$= \begin{pmatrix} e^{2t}\cos t & -e^{2t}\sin t \\ e^{2t}\sin t & e^{2t}\cos t \end{pmatrix}.$$

Next, from general prescription, we have (check it!)

$$\Phi_t = e^{tA}P = \begin{pmatrix} e^{2t}\cos t & -e^{2t}\sin t \\ e^{2t}\sin t & e^{2t}\cos t \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} ie^{(2+i)t} & -ie^{(2-i)t} \\ e^{(2+i)t} & e^{(2-i)t} \end{pmatrix}$$
$$= \left(e^{t\lambda_1}\begin{bmatrix} v_1 \end{bmatrix}, e^{t\lambda_2}\begin{bmatrix} v_2 \end{bmatrix} \right).$$

We can also check, that Φ_t is indeed the fundamental matrix solution by differentiating:

$$\frac{d\Phi_t}{dt} = \frac{d}{dt}\frac{1}{\sqrt{2}}\begin{pmatrix} ie^{(2+i)t} & -ie^{(2-i)t} \\ e^{(2+i)t} & e^{(2-i)t} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} i(2+i)e^{(2+i)t} & -i(2-i)e^{(2-i)t} \\ (2+i)e^{(2+i)t} & (2-i)e^{(2-i)t} \end{pmatrix},$$

while, on the other hand,

$$A\Phi_t = \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} ie^{(2+i)t} & -ie^{(2-i)t} \\ e^{(2+i)t} & e^{(2-i)t} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} i(2+i)e^{(2+i)t} & -i(2-i)e^{(2-i)t} \\ (2+i)e^{(2+i)t} & (2-i)e^{(2-i)t} \end{pmatrix}$$

and so $\frac{d}{dt}\Phi_t = A\Phi_t$, as desired. It remains to find the principal fundamental matrix solution, which will simply be e^{tA},

$$\Psi_t = \begin{pmatrix} e^{2t}\cos t & -e^{2t}\sin t \\ e^{2t}\sin t & e^{2t}\cos t \end{pmatrix},$$

and state transition matrix $\Psi_{t,s} = e^{(t-s)A}$,

$$\Psi_{t,s} = \begin{pmatrix} e^{2(t-s)}\cos(t-s) & -e^{2(t-s)}\sin(t-s) \\ e^{2(t-s)}\sin(t-s) & e^{2(t-s)}\cos(t-s) \end{pmatrix}.$$

2. Algebra of complex matrices

In this section we will briefly summarize some properties of space of square complex matrices of size d. In particular, we will introduce a useful notion of Hilbert-Schmidt basis, which will be of significance later on. We start with some basic facts regarding matrices. Let then a be a square matrix of size d and of complex elements, i.e.

$$A = [a_{ij}] = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1d} \\ a_{21} & a_{22} & \cdots & a_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ a_{d1} & a_{d2} & \cdots & a_{dd} \end{pmatrix}, \qquad a_{ij} \in \mathbb{C}.$$

Set of all such matrices is commonly denoted as $M_d(\mathbb{C})$ in literature. Reader might recall, that after equipping this set with two binary operations of matrix addition and multiplication by complex numbers, defined "element-wise" as

$$A + B = [a_{ij} + b_{ij}], \qquad \lambda A = [\lambda a_{ij}], \qquad \text{for all } A, B \in M_d(\mathbb{C}) \text{ and } \lambda \in \mathbb{C},$$

set $M_d(\mathbb{C})$ becomes a vector space over field $\mathbb{C}$ of dimension d^2 (why?). Moreover, if we equip the space $M_d(\mathbb{C})$ with operation of *multiplication of matrices* and add up the unary operation of Hermitian conjugation, we obtain even more elegant structure:

Theorem 6. Structure $(M_d(\mathbb{C}), \cdot, *)$, where $M_d(\mathbb{C})$ is a vector space of complex square matrices of size d, operation $\cdot$ is a matrix multiplication and $*$ stands for Hermitian conjugation, is a *noncommutative unital *-algebra* over $\mathbb{C}$.

Proof. In order to show, that it indeed is an algebra, it is sufficient to check the general axioms elaborated in Definition 5. This algebra is noncommutative (nonabelian), since one easily shows that

operation of matrix multiplication is in general not commutative, and is unital, since the natural neutral element with respect to matrix multiplication, is simply the identity matrix I. The operation of Hermitian conjugation $A \mapsto A^*$ is then also easy to show as being the involution on $M_d(\mathbb{C})$.

2.1. Hilbert space structure

Matrix space is simply yet another vector space of finite dimension over field of complex numbers, and as such, it may be given the structure of **normed space** under its own rights. Even more, there exists a well-established and commonly inner product on $M_d(\mathbb{C})$, which even makes it a Hilbert space.

Theorem 7. (Hilbert-Schmidt inner product) Let $A, B \in M_d(\mathbb{C})$. We define

$$\langle A, B\rangle_2 = \operatorname{tr} A^* B,$$

where $\operatorname{tr} A$ denotes the trace of matrix A. Then, map $(A, B) \mapsto \langle A, B\rangle_2$ is an inner product on space $M_d(\mathbb{C})$, called the *Hilbert-Schmidt inner product* or *Frobenius inner product*.

The norm, which is induced by this inner product is called the *Hilbert-Schmidt norm* or *Frobenius norm* and it can be shown, that it can be computed as

$$\|A\|_2 = \sqrt{\langle A, A\rangle_2} = \sqrt{\operatorname{tr} A^* A} = \sqrt{\sum_{i,j=1}^{d} |a_{ij}|^2}.$$

2.1.1. Hilbert-Schmidt orthonormal basis

The notion of Hilbert-Schmidt inner product allows one to introduce a natural basis in space $M_d(\mathbb{C})$, which is orthonormal with respect to this inner product. Such bases (there is infinitely many of them) are then called the Hilbert-Schmidt bases or Frobenius bases. One can show, that amongst all such bases, there always exists a one, special basis, which we will be denoting as $\{F_i\}$, which consists of mutually orthonormal and Hermitian square matrices of size d. Such basis contains exactly d^2 matrices (since we remember, that $\dim M_d(\mathbb{C}) = d^2$) and is characterized by the following properties:

1. $F_i^* = F_i$ for all $i \in \{1, \ldots, d^2\}$,
2. $F_{d^2} = \frac{1}{\sqrt{d}} I$,
3. $\operatorname{tr} F_i = 0$ for all $i < d^2$,
4. $\langle F_i, F_j\rangle_2 = \operatorname{tr} F_i F_j = \delta_{ij}$.

It can be shown that one can construct a basis satisfying the above assumptions, in such a way, that matrices F_i become either *diagonal of zero trace*, or *symmetric off-diagonal*, or *antisymmetric*. In such case the basis set $\{F_i\}$ divides into a disjoint sum $\{F_i\} = \left\{\frac{1}{\sqrt{d}} I, F_i^{\mathrm{d.}}\right\} \cup \{F_i^{\mathrm{s.}}\} \cup \{F_i^{\mathrm{a.}}\}$ such that:

1. $F_i^{\mathrm{d.}}$ are diagonal and $\operatorname{tr} F_i^{\mathrm{d.}} = 0$,
2. $F_i^{\mathrm{s.}}$ are symmetric and off-diagonal, i.e. $\left(F_i^{\mathrm{d.}}\right)^T = F_i^{\mathrm{d.}}$, $\left(F_i^{\mathrm{d.}}\right)_{jj} = 0$,
3. $F_i^{\mathrm{a.}}$ are antisymmetric, i.e. $(F_i^{\mathrm{a.}})^T = -F_i^{\mathrm{d.}}$.

For the convenience of the Reader, below we present examples of such basis in cases $d = 2$ and 3.

Example 2. The Hilbert-Schmidt basis in $M_2(\mathbb{C})$ is the following:

$$F_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad F_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \qquad F_3 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad F_4 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

Definition 12. (Pauli matrices) It is very often to work with an orthogonal, but *unnormalized* basis in $M_2(\mathbb{C})$, given in terms of *Pauli matrices* $\sigma_1, \ldots, \sigma_4$, which are simply the matrices $F_1, \ldots, F_4$ from above without the $\frac{1}{\sqrt{2}}$ factor, i.e.

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad \sigma_4 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

The Reader is encouraged to check that indeed Pauli matrices provide a basis in $M_2(\mathbb{C})$ which is Hilbert-Schmidt orthogonal, but not orthonormal.

Example 3. The Hilbert-Schmidt basis in $M_3(\mathbb{C})$ is the following:

$$F_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \qquad F_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix}, \qquad F_3 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix},$$

$$F_4 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \qquad F_5 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 0 & -i\\ 0 & 0 & 0\\ i & 0 & 0\end{pmatrix}, \qquad F_6 = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & -i\\ 0 & i & 0\end{pmatrix},$$

$$F_7 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 0\end{pmatrix}, \qquad F_8 = \frac{1}{\sqrt{6}}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -2\end{pmatrix}, \qquad F_9 = \frac{1}{\sqrt{3}}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}.$$

Checking, that both proposed bases are in fact Hilbert-Schmidt bases in appropriate matrix spaces is straightforward and is left for the Reader as an exercise.

2.2. Positive semidefinite matrices

Definition 13. (Positive semidefinite matrix) Let $A = [a_{ij}] \in M_d(\mathbb{C})$ be a Hermitian matrix, namely $A^* = A$. Then, matrix A is called *positive semidefinite* (or sometimes *positive*, for short), symbolically $A \geq 0$, if and only if for all vectors $x \in \mathbb{C}^d$ we have

$$x^* A x = \sum_{i,j=1}^{d} a_{ij}\overline{x}_i x_j \geq 0.$$

Theorem 8. The following conditions are mutually equivalent:

1. matrix $A \in M_d(\mathbb{C})$ is positive semidefinite,
2. all eigenvalues of A are real non-negative,
3. there exists matrix $B \in M_d(\mathbb{C})$ such that $A = B^*B$,
4. there exists positive semidefinite matrix C such that $A = C^2$.

Definition 14. (Convex cone) Let S be a subset of vector space V. We call S *a convex cone*, if

$$\forall x, y \in S \; \forall \, \alpha, \beta \geq 0 : \alpha x + \beta y \in S.$$

Theorem 9. Set $M_d(\mathbb{C})^+$ of all positive semidefinite matrices of size d is a convex cone, which we will be also calling simply as ***positive cone***.

Proof. Let us take two matrices $A, B \in M_d(\mathbb{C})^+$. From definition of positive semidefiniteness, we have,

that for all $x \in \mathbb{C}^d$,

$$x^*Ax \geq 0, \qquad x^*Bx \geq 0.$$

We therefore have, for any $\alpha, \beta \geq 0$,

$$x^*(\alpha A + \beta B)x = \alpha x^*Ax + \beta x^*Bx \geq 0,$$

which holds true for all vectors $x \in \mathbb{C}^d$, so $M_d(\mathbb{C})^+$ indeed is a convex cone. □

An important fact concerning positive semidefinite matrices is that they are all diagonalizable by a unitary matrix, i.e. for every positive semidefinite matrix $A \in M_d(\mathbb{C})^+$ there exists a unitary matrix U such that

$$A = UDU^*, \qquad D = \mathrm{diag}\{\lambda_1, \lambda_2, \ldots, \lambda_d\}$$

and all eigenvalues λ_i of A are non-negative, $\lambda_i \geq 0$.

2.3. Trace norm

Apart from the Hilbert-Schmidt norm, one introduces yet another norm in space of square matrices, which in very natural manner captures many key features of dynamical maps in open quantum systems theory, namely the **trace norm**. We have:

Definition 15. (Trace norm) Let $A \in M_d(\mathbb{C})$. A nonnegative function $A \mapsto \|A\|_1$ given as

$$\|A\|_1 = \mathrm{tr}\sqrt{A^*A},$$

where $\sqrt{M}$ stands for a *square root of matrix* M, is a norm on space $M_d(\mathbb{C})$, called the *trace norm*.

A somewhat peculiar construct, which appears in above definition, is without a doubt the square root of a matrix. In general, a matrix R is called the **square root of matrix** M if and only if it happens, that $R^2 = M$. It may happen, that a given matrix has even infinitely many square roots, however we will not be exploring this notion in detail, and we will focus only on positive semidefinite matrices instead. In particular, one shows[6] that the following theorem holds:

Theorem 10. (Uniqueness of square root) Let $A \in M_d(\mathbb{C})^+$, so $A = UDU^*$ for some unitary matrix U and diagonal matrix D with non-negative entries λ_i, the eigenvalues of A. Then, there exists a *unique square root* $\sqrt{A}$, which is again positive semidefinite and may be computed as

$$\sqrt{A} = U\sqrt{D}U^* = U\underbrace{\begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_d} \end{pmatrix}}_{\sqrt{D}}U^*.$$

The Reader for sure already noticed, that there is a positive semidefinite matrix A^*A appearing under the square root in definition of trace norm – therefore, computing its exact value shows no difficulty in general.

Theorem 11. (Trace norm of any matrix) Let $A \in M_d(\mathbb{C})$. Then we have

[6] This is a conclusion following from two very general result in functional analysis: the *spectral theorem* and the *spectral mapping theorem*.

$$\|A\|_1 = \sum_{i=1}^{d} \sqrt{\mu_i},$$

where numbers μ_i are the eigenvalues of matrix A^*A.

Proof. Note that matrix A^*A is, by definition, positive semidefinite and therefore Hermitian. This means that $A^*A = UDU^*$ where again U is unitary and D is diagonal and of the form

$$D = \begin{pmatrix} \mu_1 & 0 & \cdots & 0 \\ 0 & \mu_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mu_d \end{pmatrix}$$

where all $\mu_i \geq 0$. Applying Theorem 10 for matrix A^*A we have

$$\sqrt{A^*A} = U\sqrt{D}U^*.$$

Next, we use an important cyclic property of a trace, namely, for each $A, B \in M_d(\mathbb{C})$ we have

$$\operatorname{tr} AB = \operatorname{tr} BA.$$

All of this allows us to write

$$\|A\|_1 = \operatorname{tr} U\sqrt{D}U^* = \operatorname{tr} \underbrace{U^*U}_{I}\sqrt{D} = \operatorname{tr}\sqrt{D} = \operatorname{tr}\begin{pmatrix} \sqrt{\mu_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\mu_d} \end{pmatrix} = \sum_{i=1}^{d} \sqrt{\mu_i},$$

which concludes the proof. □

Theorem 12. (Trace norm of positive semidefinite matrix) Let $A \in M_d(\mathbb{C})$ be positive semidefinite. Then $\|A\|_1 = \operatorname{tr} A$.

Proof. If $A \in M_d(\mathbb{C})^+$, then in particular A is Hermitian, so it is of a form $A = UDU^*$ for some unitary U and diagonal matrix D containing nonnegative eigenvalues λ_i of A on its main diagonal. From general theory of functions on normal matrices we have $A^2 = UDU^*UDU^* = UD^2U^*$ and A^2 is also positive semidefinite; then, Theorem 10 applied for matrix A^2 yields

$$\sqrt{A^2} = U\sqrt{D^2}U^* = U\begin{pmatrix} \sqrt{\lambda_1^2} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\lambda_d^2} \end{pmatrix}U^* = U\begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{pmatrix}U^*$$

since eigenvalues of A^2 are just the squares of eigenvalues of A and every $\lambda_i \geq 0$. Utilizing again the cyclicity of trace we have

$$\|A\|_1 = \operatorname{tr}\sqrt{A^*A} = \operatorname{tr}\sqrt{A^2} = \operatorname{tr}\left[U\begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{pmatrix}U^*\right] = \operatorname{tr}\left[\underbrace{U^*U}_{I}\begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{pmatrix}\right]$$
$$= \operatorname{tr}\begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{pmatrix} = \sum_{i=1}^{d} \lambda_i = \operatorname{tr} A,$$

which is the claim. □

Example 4. We will find the trace norm of a matrix

$$A = \begin{pmatrix} 2 & 0 \\ i & -1 \end{pmatrix}.$$

First, we compute

$$A^*A = \begin{pmatrix} 2 & -i \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 2 & 0 \\ i & -1 \end{pmatrix} = \begin{pmatrix} 5 & i \\ -i & 1 \end{pmatrix}$$

and its characteristic polynomial,

$$\det(A^*A - \mu I) = \det\begin{pmatrix} 5-\lambda & i \\ -i & 1-\lambda \end{pmatrix} = (5-\lambda)(1-\lambda) - 1 = 0,$$

which we easily solve for μ, in order to find $\mu_1 = 3 + \sqrt{5}$ and $\mu_2 = 3 - \sqrt{5}$. Now it is sufficient to calculate (check it!)

$$\|A\|_1 = \sum_{i=1}^{d} \sqrt{\mu_i} = \sqrt{3+\sqrt{5}} + \sqrt{3-\sqrt{5}} = \sqrt{10}.$$

Theorem 13. For any $A \in M_d(\mathbb{C})$ it holds, that $\|A\|_2 \leq \|A\|_1$, so the trace norm dominates the Hilbert-Schmidt norm.

We will not be proving this claim.

3. Positive and completely positive maps

This section is devoted to the particularly important and distinctive class of linear maps, so-called *positive* and *completely positive maps*, which provides the main building block for the mathematics of theory of open quantum systems. Although we will be restricting our analysis – for simplicity – solely to the case of maps on finite dimensional algebras of complex square matrices, the Reader must be aware that the general concept of (completely) positive map reaches far beyond the scope given in this lecture and is itself a subject of still ongoing, intensified research. First, we will give a general idea of positivity of a map and then we will introduce a much more restrictive, yet also more tractable, case of complete positivity.

3.1. Positive maps on matrix algebras

Recall, that we have already introduced a notion of positive semidefinite matrix, i.e. a Hermitian matrix $A \in M_d(\mathbb{C})$, which satisfied condition $x^*Ax \geq 0$ for every complex vector x, or, equivalently, a Hermitian matrix of purely real, non-negative eigenvalues. We have also already shown that a set $M_d(\mathbb{C})^+$ of all such matrices is a convex cone in algebra of all square matrices. Let us then consider two, possibly distinct matrix algebras $\mathcal{A}$ and $\mathcal{B}$ and denote also by $\mathcal{A}^+$ and $\mathcal{B}^+$ convex cones of positive semidefinite matrices in both algebras. Let $T : \mathcal{A} \to \mathcal{B}$ be a linear map, which acts on matrices from $\mathcal{A}$ and returns matrices in $\mathcal{B}$. Speaking informally, map T will be called positive, if it does not affect positive semi-definiteness of matrices:

Definition 16. Map $T : \mathcal{A} \to \mathcal{B}$ is called a *positive map* if and only if $T(\mathcal{A}^+) \subseteq \mathcal{B}^+$, i.e. the set of all its values, calculated from arguments taken from a positive cone in source algebra lays inside positive cone in target algebra.

It turns out, that exploring the vast world of positive maps is a very tough task, even in case of low-dimensional algebras. Despite very series effort and extensive work done by few generations of mathematicians in both 20th and 21st century, the characterisation of set of all positive maps is far from being finalized. Fortunately, the – seemingly much more involved, yet very useful – case of *completely positive maps* can be characterized by already well-known and well-established tools; we will sketch this characterisation in Section 4.

3.2. N-positivity and complete positivity

Here we will provide a certain extension of a notion of positive map, which ultimately lead us to the notion of complete positivity, which proved itself to be extremely useful in quantum physics. We will start with so-called n-positivity, which demands from us introducing yet another operation on the set of matrices, the Kronecker product.

3.2.1. Kronecker (tensor) product of matrices

Definition 17. Let $M_{m,n}(\mathbb{C})$, $M_{r,s}(\mathbb{C})$ by linear spaces of complex matrices of a size, respectively, m by n and r by s. Take any two matrices $A \in M_{m,n}(\mathbb{C})$, $B \in M_{r,s}(\mathbb{C})$. We define the *Kronecker product* (or a tensor product) of matrices A and B to be such a matrix $A \otimes B \in M_{mr,ns}(\mathbb{C})$, that

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{pmatrix}$$

$$= \begin{pmatrix} a_{11}b_{11} & \cdots & a_{11}b_{1s} & a_{12}b_{11} & \cdots & a_{12}b_{1s} & \cdots & \cdots & a_{1n}b_{1s} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \cdots & \cdots & \vdots \\ a_{11}b_{r1} & \cdots & a_{11}b_{rs} & a_{12}b_{r1} & \cdots & a_{12}b_{rs} & \cdots & \cdots & a_{1n}b_{rs} \\ a_{21}b_{11} & \cdots & a_{21}b_{1s} & a_{22}b_{11} & \cdots & a_{22}b_{1s} & \cdots & \cdots & a_{2n}b_{1s} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \cdots & \cdots & \vdots \\ a_{21}b_{r1} & \cdots & a_{21}b_{rs} & a_{22}b_{r1} & \cdots & a_{22}b_{rs} & \cdots & \cdots & a_{2n}b_{rs} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ a_{m1}b_{r1} & \cdots & a_{m1}b_{rs} & a_{m2}b_{r1} & \cdots & a_{m2}b_{rs} & \cdots & \cdots & a_{mn}b_{rs} \end{pmatrix}.$$

Consequently, linear space of all such Kronecker products between matrices from spaces $M_{m,n}(\mathbb{C})$ and $M_{r,s}(\mathbb{C})$ will be denoted $M_{m,n}(\mathbb{C}) \otimes M_{r,s}(\mathbb{C})$. By construction of Kronecker product, it is also easy to see that a natural isomorphism

$$M_{m,n}(\mathbb{C}) \otimes M_{r,s}(\mathbb{C}) \simeq M_{mr,ns}(\mathbb{C})$$

holds. What will be of particular importance is that the block structure of $A \otimes B$ suggests, that one can interpret the Kronecker product of two matrices as an object laying in the space $M_{m,n}\big(M_{rs}(\mathbb{C})\big)$, i.e. as a m-by-n matrix with entries from the space $M_{rs}(\mathbb{C})$, i.e.

$$C = [C_{ij}]_{m\times n} \in M_{m,n}\Big(M_{r,s}(\mathbb{C})\Big), \qquad \text{where } C_{ij} \in M_{r,s}(\mathbb{C}).$$

In case of $A \otimes B$, we easily spot, that $A \otimes B = [C_{ij}]_{m\times n}$ for $C_{ij} = a_{ij}B$. In fact, one can prove that the space $M_{m,n}\Big(M_{r,s}(\mathbb{C})\Big)$ is isomorphic to $M_{mr,ns}(\mathbb{C})$ and to $M_{m,n}(\mathbb{C}) \otimes M_{r,s}(\mathbb{C})$ in result.

Example 5. We will compute the Kronecker product between two matrices of size 2,

$$A = \begin{pmatrix} 1 & 0 \\ -3 & i \end{pmatrix}, \qquad B = \begin{pmatrix} 5 & -2 \\ 2i & 0 \end{pmatrix}.$$

By definition, we have

$$A \otimes B = \begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 5 & -2 \\ 2i & 0 \end{pmatrix} & 0\begin{pmatrix} 5 & -2 \\ 2i & 0 \end{pmatrix} \\ -3\begin{pmatrix} 5 & -2 \\ 2i & 0 \end{pmatrix} & i\begin{pmatrix} 5 & -2 \\ 2i & 0 \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} \begin{pmatrix} 5 & -2 \\ 2i & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} -15 & 6 \\ -6i & 0 \end{pmatrix} & \begin{pmatrix} 5i & -2i \\ -2 & 0 \end{pmatrix} \end{pmatrix} \simeq \begin{pmatrix} 5 & -2 & 0 & 0 \\ 2i & 0 & 0 & 0 \\ -15 & 6 & 5i & -2i \\ -6i & 0 & -2 & 0 \end{pmatrix}.$$

Note, that we did not place an equality sign in the last line of the above calculation, since, mathematically, in last line we obtained two different objects: the first one is a matrix from space $M_2\big(M_2(\mathbb{C})\big)$, so it's a matrix whose entries are also matrices, whenever the last object is a 4-by-4 matrix, so an object from space $M_4(\mathbb{C})$. However, we know that spaces $M_2\big(M_2(\mathbb{C})\big)$ and $M_4(\mathbb{C})$ are isomorphic and so these two obtained matrices "are equivalent".

3.2.2. Extending maps on matrix algebras

Let now $M_d(\mathbb{C})$ and $M_n(\mathbb{C})$ be two *-algebras of complex square matrices of size d and n, respectively, and let $T : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ be any linear map. We denote by I_n the identity map on algebra $M_n(\mathbb{C})$, i.e. such a map, that for each $M \in M_n(\mathbb{C})$ we have $I(M) = M$.

We define a new map $T_n : M_n\big(M_d(\mathbb{C})\big) \to M_n\big(M_d(\mathbb{C})\big)$ by setting, for every $[A_{ij}] \in M_n\big(M_d(\mathbb{C})\big)$,

$$T_n\big([A_{ij}]\big) = (\mathrm{id}_n \otimes T)\big([A_{ij}]\big) = [T(A_{ij})],$$

or, more explicitly,

$$T_n\big([A_{ij}]\big) = \begin{pmatrix} T(A_{11}) & \cdots & T(A_{1n}) \\ \vdots & \ddots & \vdots \\ T(A_{n1}) & \cdots & T(A_{nn}) \end{pmatrix}.$$

Definition 18. (n-positive map) Let T be as above. We say that T is a *n-positive map* if and only if map T_n is positive on space $M_n\big(M_d(\mathbb{C})\big)$.

Definition 19. (Completely positive map) We say that a linear map $T : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ is *completely positive* (CP for short), if and only if it is n-positive for all $n \in \mathbb{N}$.

4. Characterisation of complete positivity

Although the definition of complete positivity is with no doubt involved and therefore may be discouraging at first, in practice it turns out that working with CP maps is much more appealing and comfortable, than it seems. In fact we have quite a number of mathematical tools available in our disposal, which provide a convenient and thorough characterisation of such maps (at least if finite-dimensional case) and in particular allow for practical, computational testing for complete positivity. We will present three of such general results, namely the Choi theorem and then the Kraus representation and Stinespring representation (in a simplified manner).

4.1. Choi theorem

Definition 20. (Choi matrix) Let $T : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ be a linear map. The block matrix C_T given by equality

$$C_T = \sum_{i,j=1}^{d} E_{ij} \otimes T\big(E_{ij}\big),$$

where matrices E_{ij} contain 1 in place (i, j) and 0 everywhere else, is called the *Choi matrix of map T*.

Theorem 14. (Choi) Let $T : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ be linear. The following conditions are mutually equivalent:

1. T is d-positive.
2. matrix C_T is positive semidefinite.
3. T is completely positive.

The Reader may find a proof of the above statement in a number of books concerning linear algebra topics, for instance in [2]. Choi's theorem allows for practical testing for complete positivity of maps on matrix algebras – in principle, to find if a given map is CP it suffices to check for definiteness (i.e. Hermiticity and non-negativity of spectrum) of its associated Choi matrix, which is a task achievable at least by numerical methods. Also, an important consequence of this theorem is that in finite dimensional setting, complete positivity is the same, as d-positivity, which is a great simplification.

Example 6. Let us consider a simple map $\phi: M_2(\mathbb{C}) \to M_2(\mathbb{C})$ defined by

$$\phi([a_{ij}]) = \begin{pmatrix} 2a_{11} & -ia_{11} - a_{12} \\ ia_{11} - a_{21} & a_{11} + a_{22} \end{pmatrix}.$$

We will check, using Choi's theorem, if this map is completely positive. For $d = 2$ there are 4 matrices E_{ij}:

$$E_{11} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad E_{21} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad E_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad E_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

The action of ϕ on them is as follows:

$$\phi(E_{11}) = \begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix}, \quad \phi(E_{21}) = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, \quad \phi(E_{12}) = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, \quad \phi(E_{22}) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

The Choi matrix is then

$$\begin{aligned} C_\phi &= E_{11} \otimes \phi(E_{11}) + E_{21} \otimes \phi(E_{21}) + E_{12} \otimes \phi(E_{12}) + E_{22} \otimes \phi(E_{22}) \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1\begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix} & 0\begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix} \\ 0\begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix} & 0\begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix} \end{pmatrix} + \begin{pmatrix} 0\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \\ 1\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \end{pmatrix} + \begin{pmatrix} 0\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} & 1\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} \\ 0\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} \end{pmatrix} \\ &+ \begin{pmatrix} 0\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & 0\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ 0\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & 1\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} \\ &= \begin{pmatrix} 2 & -i & 0 & 0 \\ i & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 2 & -i & 0 & -1 \\ i & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}. \end{aligned}$$

It remains to find spectrum of C_ϕ. This is achieved by calculating roots of the characteristic polynomial of C_ϕ:

$$\begin{aligned} \det(C_\phi - \lambda I) &= \det\begin{pmatrix} 2-\lambda & -i & 0 & -1 \\ i & 1-\lambda & 0 & 0 \\ 0 & 0 & -\lambda & 0 \\ -1 & 0 & 0 & 1-\lambda \end{pmatrix} = (-\lambda)(-1)^{3+3} \det\begin{pmatrix} 2-\lambda & -i & -1 \\ i & 1-\lambda & 0 \\ -1 & 0 & 1-\lambda \end{pmatrix} \\ &= -\lambda \cdot \left((2-\lambda)(1-\lambda)^2 - (1-\lambda) + i^2(1-\lambda)\right) = \lambda^2(\lambda-1)(\lambda-3). \end{aligned}$$

From this we immediately read the roots, i.e. eigenvalues of C_ϕ, to be $\lambda_1 = 0$ (of multiplicity 2), $\lambda_2 = 1$, $\lambda_3 = 3$. Of course, all eigenvalues are nonnegative and hence C_ϕ is positive semidefinite. According to Choi's theorem, such map ϕ is then completely positive.

4.2. Kraus and Stinespring representations

As an immediate, yet no so obvious consequence of Choi theorem is the so-called *Kraus representation* of every completely positive map. We present it as a following theorem:

Theorem 15. (Kraus representation) Let T be a completely positive map on matrix *-algebra $M_d(\mathbb{C})$. Then, there exists a family $\{V_i\} \subset M_d(\mathbb{C})$ of at most d^2 square matrices, such that for any $A \in M_d(\mathbb{C})$ we have

$$T(A) = \sum_{i=1}^{d^2} V_i A V_i^*.$$

The above is commonly called the *Kraus representation*[7] *of* T, and matrices V_i are called *Kraus operators of* T. Such representation is **not unique**. And vice versa, if a map T admits such a representation, then it is completely positive.

Below we will also mention one of the incarnations of a very deep and robust abstract result, known as the *Stinespring dilation theorem*, which in fact is the characterisation theorem for completely positive maps on (general, even infinite-dimensional) C*-algebras, making it a most important result in the entire field of CP maps. We will present it in a version, which will be useful for us in forthcoming sections devoted to open systems analysis:

Theorem 16. (Stinespring representation of a CP map) Let T be a completely positive linear map on *-algebra $M_d(\mathbb{C})$. Then, there exists an auxiliary Hilbert space $K \simeq \mathbb{C}^k$ of dimension $k \leq d^2$, a unitary operator $U : \mathbb{C}^d \otimes \mathbb{C}^k \to \mathbb{C}^d \otimes \mathbb{C}^k$ and a positive semidefinite matrix $\omega \in M_k(\mathbb{C})$ such that

$$T(A) = \mathrm{tr}_K\, U(A \otimes \omega)U^* \quad \text{for every } A \in M_d(\mathbb{C}),$$

where tr_K denotes the *partial trace* over K.

Example 7. It may be beneficial for the Reader to check that in fact, the map ϕ considered in previous example was designed to be expressible as

$$\phi(A) = V_1 A V_1^* + V_2 A V_2^*$$

for matrices $V_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $V_1 = \begin{pmatrix} 1 & 0 \\ i & 0 \end{pmatrix}$.

5. Density operator in quantum mechanics

Starting from this section, we will be focused on mathematical description of physical systems, which are – in contrast to standard, "unitary" case, which the Reader probably already is quite familiar with from the introductory course to quantum mechanics – not closed, or, in other words, are allowed to interact with some environment. Effects of such interaction have to be treated and described with the use of much more general apparatus, than the one used in quantum mechanics of isolated systems, which was entirely based on the Schrödinger equation imposed on a time-dependent normalized vector (the *state*) in some Hilbert space.

[7] Sometimes also called *Choi-Kraus representation* or even *Stinespring representation*.

Let us recall that the evolution of a state of a general isolated quantum mechanical system, i.e. a non-interacting system of total energy conserved, was characterized in terms of the famous Schrödinger equation of a form (we put $\hbar = 1$ for brevity)

$$\frac{d}{dt}\psi(t) = -iH\psi(t),$$

where $\psi(t) \in H$ is a vector of norm 1 in some (in most cases, separable) Hilbert space, called the state vector, and H stands for a Hamiltonian (the energy operator) of a given system. In most simple case of time-independent H, the solution of above equation was simply given as

$$\psi(t) = U_{t,t_0}\psi(t_0),$$

where $U_{t,t_0} = e^{-iH(t-t_0)}$ is a unitary operator, transforming state from some previous moment t_0 to some later moment $t \geq t_0$, called the *evolution operator*. We assume the Reader is already well familiar with this notion and so we will not be exploring the evolution of such sort in general.

5.1. Definition and properties

Below we present a very general, broad definition of a density operator, which is well-suited for describing all physical systems, even in infinite-dimensional setting. Later on we will, for simplicity, focus on a finite-dimensional case only, however a majority of our analysis will still more or less apply to infinite-dimensional case, possibly with some technicalities involved. First, we briefly sketch a concept of a trace class operator. Let H stand for some complex, separable Hilbert space spanned by a countable orthonormal basis $\{e_n\}$ and let $B(H)$ denote the space[8] of all bounded, linear operators on H. There is a special subspace of operators in $B(H)$, which have a finite *trace*, i.e. such that a series

$$\operatorname{tr} T = \sum_n \langle e_n, Te_n \rangle$$

converges in $\mathbb{C}$; such operators are called **trace class operators**. The subspace in $B(H)$ of all such operators, here denoted $B_1(H)$, simply called *the trace class*, becomes a Banach space after equipping it with a trace norm

$$\|T\|_1 = \operatorname{tr}\sqrt{T^*T}.$$

Note, that a notion of a trace norm used in the above context is determined by the very same general formula, as in the matrix case in Section 2.3. The existence of a square root of an operator is also assured by the fact, that T^*T is a *positive semi-definite operator*, i.e. that it satisfies $\langle x, Tx \rangle \geq 0$ for all $x \in H$, same as in matrix case (equivalently, we say that an operator $A \in B(H)$ is positive semidefinite if and only if it is self-adjoint, $A = A^*$, and its spectrum lays on the nonnegative semiaxis). One can show that the trace class $B_1(H)$ is, in fact, the predual space for whole $B(H)$, and also, that it is a dual of a space $K(H)$ of all compact operator on H. Moreover, a general, set-theoretic inclusion $B_1(H) \subset K(H) \subset B(H)$ holds.

Definition 21. (The density operator) Let H be some separable Hilbert space, possibly infinite-dimensional. A trace class operator $\rho \in B_1(H)$, which is *positive semi-definite* and of *trace* 1, will be called the *density operator*.

Let then ρ be a density operator. We stress here three key features of such:

Theorem 17. The following statements hold:

[8] After equipping $B(H)$ with Hermitian conjugation, $T \mapsto T^*$, it becomes a *-algebra similarly to matrix case, and after adding an *operator norm*, $\|T\| = \sup_{\|x\| \leq 1} \|Tx\|$, it becomes a so-called *C*-algebra*.

1. Density operator ρ is of trace norm 1, i.e. $\|\rho\|_1 = 1$.
2. Each density operator ρ admits a (nonunique) decomposition into a convex combination of projection operators onto subspaces in H, i.e.

$$\rho = \sum_j p_j P_j,$$

where $p_j \in [0,1]$, $\sum_j p_j = 1$ and P_j are projection operators in H. Moreover, one can always find a decomposition, such that all P_j project onto mutually orthogonal subspaces in H (i.e. such, that $P_j P_k = \delta_{jk} P_k$, $\mathrm{im}\, P_j \perp \mathrm{im}\, P_k$ for $j \neq k$ and $H = \bigoplus_j \mathrm{im}\, P_j$.

3. Spectrum of density operator is countable, consists of *eigenvalues* and may contain only 0 as its limit point. If space H in question is infinite-dimensional, then 0 necessarily lays in the spectrum and so ρ becomes noninvertible.

5.2. Interpretation and motivation

The usefulness of density operator lays mainly in description of so-called *mixed states*, which are quantum-mechanical analogues of *statistical ensembles*. The notion of density operator also appears very naturally in description of systems interacting with each other; it turns out, that in such case, a traditional approach based solely on state vectors simply is not suitable enough for, for instance, computing expectation values of certain observables.

Recall, that in the traditional approach, constituted by postulates of quantum mechanics, the whole information about the physical system was contained in the state vector $\psi \in H$, i.e. knowing ψ, we had access to the complete information about the system. In general scenario, however, we simply have no such luxury because of – for example – large number of individual particles involved, or present, in the entire system. So, the one feasible way of justification for the need of density operator approach is the statistical one: one may say that the only information which we have access to, is the general statistics, or a *probability distribution*, of quantum states present in the system, so the information overall is simply not complete.

5.2.1. Expectation values and statistical ensembles

As a thought model, let us consider a system consisting of large number of individual subsystems, let them be particles inside a box, such that the i-th particle is in some quantum state ψ_i. The important ingredient of our analysis is the assumption that we do not *a priori* know which particle is in which state, and the only information we have access to is the probability distribution of finding the random particle in a box in given state. Let us assume we would like to find the expectation value of some observable A, measured on a randomly selected particle from the box. If there was only one particle, the obvious expectation value would be simply

$$\langle A \rangle = \langle \psi_1, A\psi_1 \rangle,$$

according to postulates of quantum mechanics. If, however, there is, say N distinct particles in the box, each one in some state ψ_i occurring with **probability** p_i, then one has to account for the uncertainty of choosing the i-th state from the box, i.e. the expectation value of A must be given as an **expectation of different expectation values** $\langle \psi_i, A\psi_i \rangle$, appearing with probability p_i, namely one has to compute

$$\langle A \rangle = \sum_{i=1}^{N} p_i \langle \psi_i, A\psi_i \rangle.$$

Such expression contains in fact two very distinct procedures of calculating the expectation value: the *statistical one* (or over a probability distribution) and a *quantum mechanical one* (with respect to given state vector). Now, let us introduce an operator

$$P_i = \langle \psi_i, \cdot \rangle \psi_i,$$

which acts on vectors[9] $x \in H$ as $P_i x = \langle \psi_i, x \rangle \psi_i$. The Reader is encouraged to verify that such P_i is an *orthogonal projection operator* onto a *one-dimensional subspace in H spanned by vector ψ_i*. Now, recall, that in case of general operator T of a form $T = \langle \phi, \cdot \rangle \varphi$ for $\phi, \varphi \in H$ one has

$$\operatorname{tr} T = \langle \phi, \varphi \rangle.$$

This yields, by self-adjointness of A,

$$\langle \psi_i, A\psi_i \rangle = \operatorname{tr}[\langle A\psi_i, \cdot \rangle \psi_i] = \operatorname{tr}[\langle \psi_i, A \cdot \rangle \psi_i] = \operatorname{tr} P_i A,$$

and therefore

$$\langle A \rangle = \sum_{i=1}^{N} p_i \langle \psi_i, A\psi_i \rangle = \sum_{i=1}^{N} p_i \operatorname{tr} P_i A = \operatorname{tr}\left[\left(\sum_{i=1}^{N} p_i P_i\right) A\right].$$

Now, object $\sum_{i=1}^{N} p_i P_i$ is clearly a convex combination of projection operators, and so is a **density operator**. Therefore, we obtain, that the expectation value of observable A, calculated over a statistical ensemble of vector states ψ_i appearing with probability p_i, is the expression

$$\langle A \rangle = \operatorname{tr} \rho A.$$

The above construction, despite being much simplified, presents the most direct approach to the concept of density operator as a purely statistical object which allows for description of physical systems without access to full information about its constituents, i.e. mixtures of different quantum states. From this point of view, it seems natural and justified to introduce the following nomenclature:

Definition 22. (Pure states and mixed states) If a quantum-mechanical system is described with a normalized vector ψ in some Hilbert space, we say that it is in a **pure state**. If it is described as a statistical mixture (ensemble) by some density operator ρ, we say it is in a **mixed state**.

A common practice is to refer directly to ψ as a *pure state*, and to ρ as a *mixed state*. Of course, from its very definition and construction, density operator ρ behaves just like any other self-adjoint (or Hermitian, in finite dimension) trace class operator on Hilbert space and as such, may be analysed by all known, functional-analytic methods. We stress that if, in a given situation, our density matrix is simply just a one projection operator onto a one-dimensional subspace spanned by vector ψ, i.e.

$$\rho = P = \langle \psi, \cdot \rangle \psi,$$

then this means that the system is in a pure state ψ. In such case, density matrix ρ is also referred to as a *pure state*. Below we also give the Reader an important mathematical result, which allows to check for system's purity:

Theorem 18. It holds that $\operatorname{tr} \rho^2 \leq \operatorname{tr} \rho = 1$. Additionally, ρ is a pure state if and only if $\operatorname{tr} \rho^2 = 1$.

5.2.2. Density operators as reduced states of subsystems

There is yet another scenario, where the density operator appears in very natural manner, almost automatically. Even more, in a situation which we briefly describe below, the appearance of density operator is completely inevitable. Namely, let us consider a large physical system $\mathcal{S}$, which consists of two separate subsystems $\mathcal{A}$ and $\mathcal{B}$, which are allowed to interact with each other. Let us assume, that states of both subsystems are described by two Hilbert spaces $H_{\mathcal{A}}$ and $H_{\mathcal{B}}$ and moreover, that the system $\mathcal{B}$ is much larger then $\mathcal{A}$, so $\mathcal{B}$ may be considered as an "environment" from point of view of observers in $\mathcal{A}$. Typically, we have no control over the environment nor access to any complete

[9] Using the *bra-ket* (Dirac) *notation*, operator P_i may be written as $|\psi_i\rangle\langle\psi_i|$.

information about state of $\mathcal{B}$, so we will have to somehow "rule out" the environment from the analysis at certain point. We will be focusing on subsystem $\mathcal{A}$ as a system of interest.

We assume that a whole, combined system $\mathcal{A}+\mathcal{B}$ is isolated, so its quantum mechanical state is pure. According to postulates of quantum mechanics, this state is given by some normalized vector Ψ in a composite Hilbert space $H_{\mathcal{AB}} = H_{\mathcal{A}} \otimes H_{\mathcal{B}}$. Assuming, that space $H_{\mathcal{B}}$ is separable, we can always find some orthonormal basis $\{\xi_n\}$ spanning $H_{\mathcal{B}}$. Then, one easily shows that vector Ψ has a form

$$\Psi = \sum_n c_n \psi_n \otimes \xi_n,$$

where c_n are some complex coefficients and ψ_n are some normalized (not necessarily orthogonal!) vectors in $H_{\mathcal{A}}$. The Reader may check that coefficients c_n are in fact probability amplitudes of finding the environment $\mathcal{B}$ in one of its basis states ξ_n and they must fulfil $\sum_n |c_n|^2 = 1$.

Now, lets assume we want to perform a measurement of some observable A only on subsystem $\mathcal{A}$, so we want to calculate an expectation value of some self-adjoint operator A acting on $H_{\mathcal{A}}$. In language of composite Hilbert space $H_{\mathcal{A}} \otimes H_{\mathcal{B}}$, such observable is expressed as an operator $\hat{A} = A \otimes I_{\mathcal{B}}$, where $I_{\mathcal{B}}$ is the identity operator in $H_{\mathcal{B}}$ (such structure is justified, since we "do nothing" on the part $\mathcal{B}$ and our observable acts only on part $\mathcal{A}$ of the whole state). We then calculate

$$\begin{aligned}\langle \hat{A} \rangle &= \langle \Psi, \hat{A}\Psi \rangle = \left\langle \sum_n c_n \psi_n \otimes \xi_n \,, (A \otimes I_{\mathcal{B}}) \left(\sum_m c_m \psi_m \otimes \xi_m \right) \right\rangle \\ &= \sum_{n,m} \overline{c_n} c_m \langle \psi_n \otimes \xi_n, (A\psi_m) \otimes \xi_m \rangle = \sum_{n,m} \overline{c_n} c_m \langle \psi_n, A\psi_m \rangle \langle \xi_n, \xi_m \rangle \\ &= \sum_n |c_n|^2 \langle \psi_n, A\psi_n \rangle,\end{aligned}$$

which comes easily from orthonormality of vectors ξ_n and properties of inner product in tensor product spaces. However, we see, that performing the very same steps as before, we can, after defining projections $P_n = \langle \psi_n, \cdot \rangle \psi_n$, recast the last expression into

$$\sum_n |c_n|^2 \langle \psi_n, A\psi_n \rangle = \operatorname{tr}\left[\left(\sum_n |c_n|^2 P_n \right) A \right] = \operatorname{tr} \rho A,$$

where suddenly a density operator ρ of a form

$$\rho = \sum_n |c_n|^2 P_n = \sum_n |c_n|^2 \langle \psi_n, \cdot \rangle \psi_n$$

appeared almost out of nowhere. We also notice that this density operator describes subsystem $\mathcal{A}$ only. Such an object is then called the **reduced density operator** and, speaking mathematically, appears as an effect of procedure of so-called *partial trace*.

5.2.3. Time evolution of density operators in isolated systems

Remember, that the dynamics of isolated systems in pure states, i.e. expressed entirely by a state vector from a Hilbert space, was characterized in terms of the famous Schrödinger equation, which involved an energy operator, the Hamiltonian. One may then ask a question what is the natural equation of motion for a density operator, i.e. a mixed state of an isolated system? We claim the answer to be the following:

Theorem 19. Let ρ_t be the density operator of an isolated system with a constant Hamiltonian H. Then, ρ_t is subject to **the von Neumann equation** of motion of a form

$$\frac{d\rho_t}{dt} = -i[H, \rho_t],$$

where $[A, B] = AB - BA$ stands for the commutator of operators A and B. In consequence, the time dependence of ρ_t is given by expression

$$\rho_t = e^{-iH(t-t_0)}\rho_{t_0}e^{iH(t-t_0)},$$

where ρ_{t_0} is an initial density operator.

Proof. We prove this theorem backwards, i.e. we start with time dependence of ρ_t. First, we put ρ_t in a form of a convex combination of projections onto one-dimensional eigenspaces of ρ_t, given by some time-dependent eigenvectors $\phi_n(t)$, i.e. we have

$$\rho_t = \sum_n p_n(t)\langle\phi_n(t),\ \cdot\rangle\phi_n(t),$$

where $0 \leq p_n(t) \leq 1$ and $\sum_n p_n(t) = 1$. Since our system is isolated from the environment, it is reasonable to make a simplifying assumption, that *the probability distribution (or statistical weights) of pure states, encoded in the mixed state in terms of coefficients $p_n(t)$, remains constant in time*. This means, that ρ_t should be rather given as

$$\rho_t = \sum_n p_n\langle\phi_n(t),\ \cdot\rangle\phi_n(t),$$

where all the time dependence is present only in projections $\langle\phi_n(t),\ \cdot\rangle\phi_n(t)$. Since we know that vectors $\phi_n(t)$ evolve freely in time, their time dependence must be entirely expressed in terms of the unitary evolution operator,

$$\phi_n(t) = U_{t,t_0}\phi_n(t_0) = e^{-iH(t-t_0)}\phi_n(t_0),$$

which means, that

$$\begin{aligned}\rho_t &= \sum_n p_n \left\langle U_{t,t_0}\phi_n(t_0),\ \cdot\right\rangle U_{t,t_0}\phi_n(t_0)\\ &= U_{t,t_0}\left(\sum_n p_n \left\langle \phi_n(t_0), U^*_{t,t_0}\cdot\right\rangle\phi_n(t_0)\right)\\ &= U_{t,t_0}\rho_{t_0}U^*_{t,t_0},\end{aligned}$$

where we introduced the initial density operator $\rho_{t_0} = \sum_n p_n \langle\phi_n(t_0),\ \cdot\rangle\phi_n(t_0)$. This proves the second part of the theorem. To show the first part, simply compute

$$\frac{d\rho_t}{dt} = \frac{d}{dt}U_{t,t_0}\rho_{t_0}U^*_{t,t_0}$$

and use the fact, that operator U_{t,t_0} is nothing more, then a **principal fundamental matrix solution** of the Schrödinger equation (compare Section 1.3.3!) i.e. that it satisfies

$$\frac{dU_{t,t_0}}{dt} = -iHU_{t,t_0}, \qquad U_{t,t} = I.$$

The remaining computation is easy and left to the Reader. □

6. Open quantum systems

Having discussed all necessary mathematical ingredients, such as complete positivity of maps, trace norm and the general concept of density operator, we are now equipped for introducing the Reader to the vast and highly successful theory of open quantum systems. Therefore, in the hereby section

we will briefly sketch the general model of an open system and its evolution. From now on, however, we will be focusing on describing finite-dimensional systems only, such that the density operator, the dynamics of which we will be trying to describe, becomes a Hermitian, positive semidefinite matrix of trace 1, called the **density matrix**. Our ultimate goal will be to provide a characterisation of time evolution of such a matrix and to develop the so-called Master Equation (in Markovian approximation).

6.1. Microscopic model of open quantum system

We start with a model of an open quantum system. We will be considering a physical system S, which is described by a d-dimensional Hilbert space $\mathbb{C}^d$ and a time-independent Hamiltonian H. This system is allowed to interact with a much larger system E, here called the environment, which is then also described by some (possibly infinite-dimensional) Hilbert space $\mathcal{H}_E$ and Hamiltonian H_E. Those two systems are allowed to interact with each other, and the interaction Hamiltonian is given as a general expression

$$H_{\text{int}} = \sum_{\alpha} S_\alpha \otimes R_\alpha,$$

where $\{S_\alpha\}$ and $\{R_\alpha\}$ are families of linear operators, acting on Hilbert spaces of subsystems S and E, respectively (operators S_α are therefore simply some complex square matrices of size d).

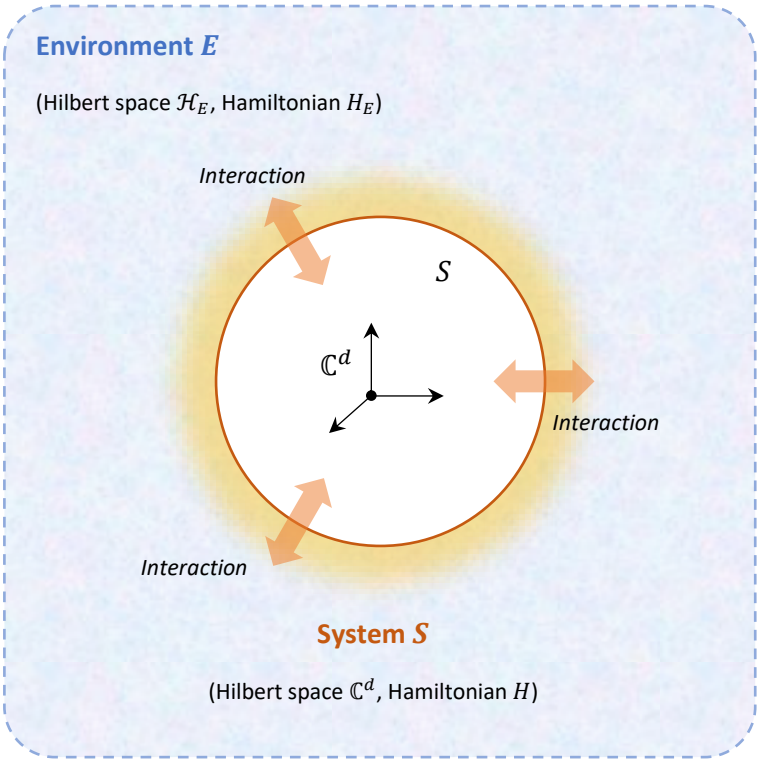

Fig. 1. A general model of open quantum system S, immersed in environment E. Both systems are allowed to interact via interaction Hamiltonian H_{int}. Hilbert space of system S is of finite dimension d, while Hilbert space of the environment, $\mathcal{H}_E$, can be infinite dimensional.

6.2. Evolution of open quantum system as CPTP map

We are now interested in describing only the evolution of subsystem S, since the general environment is pretty much inaccessible for us, as a whole, or even of no interest or practical advantage. In Section

5.2.2 it was argued that the state of a subsystem S of a combined system will in general be a **mixed state**, described by some density matrix. We are, therefore, interested in time dependence of a density matrix ρ_t of subsystem S, namely we seek for an exact form of function $t \mapsto \rho_t$.

However, if one considers at first the entire combined system $S + E$, then – provided the environment is big enough – one can expect that such is an **isolated system** and therefore it undergoes an evolution determined by *von Neumann equation*, as we argued in Theorem 19 in Section 5.2.3.

Let then σ_t be a density operator of a system $S + E$. Let also

$$H_{SE} = H \otimes I_E + I_S \otimes H_E + H_{\text{int}}$$

be the Hamiltonian of $S + E$. Since operator σ_t satisfies von Neumann equation of a form

$$\frac{d}{dt}\sigma_t = -i[H_{SE}, \sigma_t],$$

we immediately have (we put $t_0 = 0$ for convenience)

$$\sigma_t = e^{-iH_{SE}t}\sigma_0 e^{iH_{SE}t}.$$

Now, since we want to focus solely on the subsystem S, we have to average over all possible states of the environment, or, to perform the partial trace over space $\mathcal{H}_E$. The result of such partial tracing will be the reduced density matrix ρ_t of subsystem S:

$$\rho_t = \text{tr}_E\, \sigma_t = \text{tr}_E\, e^{-iH_{SE}t}\sigma_0 e^{iH_{SE}t},$$

where the initial density operator σ_0 of system $S + E$ must be a function of initial density matrix ρ_0 of our system of interest, $\sigma_0 = \zeta(\rho_0)$, where ζ is commonly assumed to be linear[10]. We therefore clearly see that the dependence $t \mapsto \rho_t$ is expressed in terms of some linear map Λ_t, which acts on the initial density matrix ρ_0 and produces a density matrix ρ_t in some given later time $t \geq 0$,

$$\rho_t = \text{tr}_E\, e^{-iH_{SE}t}\zeta(\rho_0)e^{iH_{SE}t} = \Lambda_t(\rho_0).$$

Such a map Λ_t will determine the evolution of reduced density matrix of subsystem S and is therefore called the **quantum dynamical map**. What are key properties of Λ_t?

1. First of all, putting $t = 0$ we have to return to the very start of the evolution, or obtain an initial density matrix, $\Lambda_0(\rho_0) = \rho_0$, so we have
$$\Lambda_0 = \text{id}.$$
2. Second, ρ_t must remain a density matrix at all times $t \geq 0$, so Λ_t in particular must preserve its trace norm and positive semidefiniteness. From this, we imply that Λ_t must be a **positive, trace preserving map** on $M_d(\mathbb{C})$ for all $t \geq 0$.

It turns out, that assuming that Λ_t is merely o positive map, is not enough and one can justify the necessity of imposing even stronger property – of complete positivity. Namely, let us assume that there exists, somewhere in vicinity of subsystem S, some additional n-dimensional system A, where $n > 0$, sometimes called *the ancilla*, which is distinct from the environment (however could be also surrounded by it) and which interacted with our system S at some moment in the past, say at $t = 0$. This means that the joint state $\sigma_0 \in M_d(\mathbb{C}) \otimes M_n(\mathbb{C})$ of system $S + A$ is now **entangled**, i.e. it can not be expressed as a tensor product of separate states of both systems S and A.

Assume, for simplicity, that the ancilla is so trivial, that its own Hamiltonian is 0. This means, that any dynamical map $\mathcal{N}_t$ of density operator of the ancilla must by the identity, $\mathcal{N}_t = \text{id}$, on ancilla's algebra $M_n(\mathbb{C})$, i.e. a reduced density operator of A does not change at all. Since systems S and A were interacting only for short time (just enough to establish correlations and entangled joint state between

[10] See R. Alicki: *Comment on "reduced dynamics need not be completely positive,"* Phys. Rev. Lett. **75**, 3020 (1995).

them) and no interaction occurred at any later time $t > 0$, the joint density matrix σ_t of system $S + A$ must be of a form

$$\sigma_t = (\mathcal{N}_t \otimes \Lambda_t)(\sigma_0) = (\mathrm{id}_n \otimes \Lambda_t)(\sigma_0),$$

where id_n is the identity map on algebra $M_n(\mathbb{C})$, i.e. it is given by a joint dynamical map of a **product structure**: here, the id_n is a trivial part of the evolution, which acts only on the ancilla, while Λ_t is the dynamical map of S we seek for. What must be stressed here is that **the product structure of such dynamic is justified only if subsystems A and S do not interact with each other**, which is the case here. But such an extended dynamical map $\mathrm{id}_n \otimes \Lambda_t$ must also be a *positive map* on joint algebra $M_n(\mathbb{C}) \otimes M_d(\mathbb{C})$ in order for σ_t still to be a density matrix, i.e. Λ_t must be n-positive at all times (compare with Section 3.2). Such argument can be then raised *regardless of a choice of the ancilla and its dimension* n. **In other words, map Λ_t must be n-positive for all $n \in \mathbb{N}$, or completely positive as was defined in Section 3.2.** This, in the end, allows us to define a notion of a dynamical map, which is well-suited for the open quantum systems theory:

Definition 23. (Quantum dynamical map) Let $\{\Lambda_t : t \geq 0\}$ be a family of linear maps, defined on matrix *-algebra $M_d(\mathbb{C})$. We call this family *the quantum dynamical map* if and only if:

1. $\Lambda_0 = \mathrm{id}$,
2. Λ_t is completely positive for all $t \geq 0$,
3. Λ_t is trace preserving for all $t \geq 0$, which means that $\mathrm{tr}\,\Lambda_t(\rho) = \mathrm{tr}\,\rho$ for all $\rho \in M_d(\mathbb{C})$.

Shortly, we will be referring to a completely positive and preserving map as a **CPTP map**.

An especially important feature of quantum dynamical maps is that they tend to move initially separated density matrices closer together after some time, or that they decrease *distinguishability* of mixed states. This "distinguishability" must be understood in a sense of a *trace distance* between matrices in Banach space $(M_d(\mathbb{C}), \|\cdot\|_1)$:

Theorem 20. (Contractivity) Every quantum dynamical map $\{\Lambda_t : t \geq 0\}$ is a trace norm *contraction* on the subspace of all Hermitian matrices in $M_d(\mathbb{C})$, i.e. for every $t \geq 0$ and every $\rho_1, \rho_2 \in M_d(\mathbb{C})$ such, that $\rho_1 = \rho_1^*$ and $\rho_2 = \rho_2^*$, we have

$$\|\Lambda_t(\rho_1) - \Lambda_t(\rho_2)\|_1 \leq \|\rho_1 - \rho_2\|_1.$$

Proof. Let us denote $\rho = \rho_1 - \rho_2$. It is still a Hermitian matrix, so in particular it is diagonalizable and may be put in a form

$$\rho = \sum_{i=1}^{d} \lambda_i P_i,$$

where $\lambda_i \in \mathbb{R}$ are its eigenvalues and P_i are orthogonal projections onto one-dimensional eigenspaces, spanned by eigenvectors of ρ. The eigenvalues, although real, can be both positive, 0, and negative. We then break up this sum into two sums over nonnegative and negative eigenvalues:

$$\rho = \sum_{i=1}^{d} \lambda_i P_i = \sum_{\lambda_i \geq 0} \lambda_i P_i + \sum_{\lambda_i < 0} \lambda_i P_i = \sum_{\lambda_i \geq 0} \lambda_i P_i - \sum_{\lambda_i < 0} (-\lambda_i) P_i.$$

Let us denote the two resulting sums by

$$\rho_+ = \sum_{\lambda_i \geq 0} \lambda_i P_i\,, \qquad \rho_- = \sum_{\lambda_i < 0} (-\lambda_i) P_i,$$

such that $\rho = \rho_+ - \rho_-$. The Reader may verify that both obtained matrices $\rho_\pm$ are positive semidefinite. The Hermitian matrix ρ was then split up into a difference of positive semidefinite

matrices (in fact, every Hermitian matrix, or a self-adjoint linear operator, can be split in that way). Let us now compute the trace norm of such matrix:

$$\|\rho\|_1 = \|\rho_+ - \rho_-\|_1 = \operatorname{tr}\sqrt{(\rho_+ - \rho_-)^*(\rho_+ - \rho_-)} = \operatorname{tr}\sqrt{\rho_+^2 + \rho_-^2 - \rho_-\rho_+ - \rho_+\rho_-}$$
$$= \operatorname{tr}\sqrt{\rho_+^2 + \rho_-^2},$$

where we employed Hermiticity of ρ and the fact, that $\rho_-\rho_+ = \rho_+\rho_- = 0$ (verify it!). Next, we note that

$$\rho_+^2 + \rho_-^2 = \sum_{\lambda_i \geq 0} \lambda_i^2 P_i + \sum_{\lambda_i < 0} (-\lambda_i)^2 P_i = \sum_{\lambda_i \geq 0} \lambda_i^2 P_i + \sum_{\lambda_i < 0} \lambda_i^2 P_i = \sum_{i=1}^{d} \lambda_i^2 P_i = \rho^2,$$

which is a positive semidefinite matrix. Therefore, according to Section 2.3, the trace norm we calculate is

$$\|\rho\|_1 = \operatorname{tr}\sqrt{\rho^2} = \sum_{i=1}^{d}\sqrt{\lambda_i^2} = \sum_{i=1}^{d}|\lambda_i| = \underbrace{\sum_{\lambda_i \geq 0}\lambda_i}_{\operatorname{tr}\rho_+} + \underbrace{\sum_{\lambda_i < 0}(-\lambda_i)}_{\operatorname{tr}\rho_-} = \operatorname{tr}\rho_+ + \operatorname{tr}\rho_-.$$

However, since ρ_+ and ρ_- are positive semidefinite, we have, by Theorem 12, that *their traces are equal to their trace norms*, i.e.

$$\|\rho\|_1 = \operatorname{tr}\rho_+ + \operatorname{tr}\rho_- = \|\rho_+\|_1 + \|\rho_-\|_1.$$

Let us now look at the $\Lambda_t(\rho)$. We have, by linearity, that

$$\|\Lambda_t(\rho)\|_1 = \|\Lambda_t(\rho_+ - \rho_-)\|_1 \leq \|\Lambda_t(\rho_+)\|_1 + \|\Lambda_t(\rho_-)\|_1,$$

where me employed the *triangle inequality*. Map Λ_t is positive, so matrices $\Lambda_t(\rho_\pm)$ are positive semidefinite; this yields, by the trace preservation condition,

$$\|\Lambda_t(\rho_\pm)\|_1 = \operatorname{tr}\Lambda_t(\rho_\pm) = \operatorname{tr}\rho_\pm = \|\rho_\pm\|_1,$$

which is an important property of quantum dynamical maps: all positive (not necessarily completely positive) and trace preserving maps are isometries on a subset of positive semidefinite matrices of trace one. The last equality now allows us to write

$$\|\Lambda_t(\rho)\|_1 \leq \|\Lambda_t(\rho_+)\|_1 + \|\Lambda_t(\rho_-)\|_1 = \|\rho_+\|_1 + \|\rho_-\|_1 = \|\rho\|_1,$$

i.e. $\|\Lambda_t(\rho)\|_1 \leq \|\rho\|_1$ for all Hermitian matrices ρ, which is the claimed result. □

7. Markovian dynamical maps

Having briefly sketched a general theory of open quantum system, its reduced density matrix and a physical justification standing behind the structure of its evolution, we now focus solely on the best explored and definitely most successful, up to now, approach to open systems based on the Markovian approximation. In what fallows we will describe what it means that a system undergoes the Markovian evolution and define it mathematically. This will ultimately lead to the very elegant and powerful result of *Lindblad-Gorini-Kossakowski-Sudarshan Master Equation*, i.e. an equation of motion of a reduced density matrix of open system, which structure guarantees that the resulting evolution of the system will be given as a Markovian CPTP map.

In fact, our approach to Markovian dynamical maps will be divided into two main parts. The first part, which we will explore in this section, will tend to be purely mathematical and will provide a very broad, "algebraic" result characterizing Markovian evolution in general. The second part, which we will elaborate on in Section 8, will be focused on much more "physical" approach to quantum dynamics

and will present a quite standard, so to say "microscopic" derivation of Master Equation under some additional assumptions; such derivation will ultimately lead us to the virtually same result as in the first part.

7.1. What is Markovianity?

We start with a general and not-so-formal concept of Markovianity. Loosely speaking, an evolution of some system will be called *Markovian*, or will possess a *Markov property*, if given the state of a system in a present time, say t_0, the state in any future time $t > t_0$ may depend only on the state in time t_0 and not on the history, i.e. not on states in times $t < t_0$. Then, a process possessing the Markov property will be "memoryless" in a sense. Assumption of Markovianity is a very strong one, however real physical examples show that it is perfectly reasonable to treat many naturally occurring processes as Markovian or approximate them by some Markovian process with very good result. In particular, one can almost always treat an evolution of systems, which interact with large, external reservoirs (with many internal degrees of freedom) as approximately Markovian. This is justified that if a reservoir (environment) which the system of interest interacts with is large enough, the internal correlations established between system and the reservoir through mutual interactions tend to vanish really rapidly and the reservoir remains unperturbed by the system; this ultimately lead to decrease of the information about the history of the system's state and to Markovianity of its evolution in the end.

Unfortunately, fully expressing and understanding the notion of a Markovian process is possible only with application of a general theory of stochastic processes and lays way beyond the scope of this lecture. We also note here, that in literature one may find at least a few of different, and not always mutually compatible, definitions of Markovian evolution. We therefore adapt a following, elegant and widespread definition based on divisibility of quantum dynamical maps:

Definition 24. (Markovian evolution) Let $\{\Lambda_t : t \geq 0\}$ be a quantum dynamical map, i.e. a family of CPTP maps defined as in Section 6.2. We call this family *Markovian* if and only if it is *CP-divisible*, which means that for any $t \geq 0$ and any $s \in [0, t]$ there exits a propagator $V_{t,s}$, i.e. such a map that

$$\Lambda_t = V_{t,s}\Lambda_s$$

and that $V_{t,s}$ is a **CPTP map** for every choice of parameters (t, s).

Now, note that if Λ_s is an *invertible* map, which in fact is very often a case, then one can define the propagator of Λ_t as

$$V_{t,s} = \Lambda_t \Lambda_s^{-1}.$$

Assume now $\{\Lambda_t : t \geq 0\}$ is Markovian (CP-divisible). Then, for any choice of $t \geq 0$, a map Λ_s may also be presented with application of a propagator as $\Lambda_s = V_{s,u}\Lambda_u$ for arbitrarily chosen $u \in [0, s]$. This yields, that

$$\Lambda_t = V_{t,s}\Lambda_s = V_{t,s}V_{s,u}\Lambda_u = V_{t,u}\Lambda_u,$$

so propagators of CP-divisible evolutions undergo a composition rule

$$V_{t,u} = V_{t,s}V_{s,u}$$

for any choice of $t, s, u \geq 0$ such that $u \leq s \leq t$ and both $V_{t,s}$ and $V_{s,u}$ are CPTP maps. Also, putting $t = s$ we notice

$$\Lambda_t = V_{t,t}\Lambda_t$$

which means $V_{t,t} = \mathrm{id}$. We then see a strong resemblance between propagator $V_{t,s}$ of quantum dynamical map and the notion of a **state transition matrix** (and Chapman-Kolmogorov identities) from theory of linear ODEs described in Section 1.3.3. In fact, this is precisely the case, at least for Markovian evolution.

7.2. Markovian Master Equation

The hallmark of Markovianity, as described in the last section, is that Markovian evolutions are determined by linear, differential equations – the Master Equations – which are "local in time", so to say. Let us assume that we have some open quantum system, which is described by a time-dependent density matrix ρ_t of size d and that this matrix undergoes a completely positive and trace preserving evolution

$$\rho_t = \Lambda_t(\rho_0),$$

where $\{\Lambda_t : t \geq 0\}$ is a **Markovian (CP-divisible) quantum dynamical map** and ρ_0 stands for some initial density matrix. In order to avoid some troublesome mathematical discussion, we will be restricting ourselves only to differentiable maps, i.e. we will assume the function $t \mapsto \Lambda_t$ is smooth enough[11].

We will be seeking for an equation of motion for ρ_t in a form

$$\frac{d\rho_t}{dt} = L_t(\rho_t),$$

where $L_t \in B\big(M_d(\mathbb{C})\big)$ is a time-dependent, linear map acting on algebra $M_d(\mathbb{C})$. Such an equation of motion for density matrix is commonly called the **Master Equation** in literature.

Our goal will be to present a formal construction of map L_t, Namely, we will present a (partial) proof of a following, beautiful result jointly achieved by G. Lindblad, V. Gorini, A. Kossakowski and E. C. G. Sudarshan:

Theorem 21. The quantum dynamical map $\{\Lambda_t : t \geq 0\}$ representing an evolution of density matrix ρ_t of size d is Markovian (CP-divisible) if and only if there exists a time-dependent Hermitian matrix H_t and a finite family of time-dependent matrices $\{X_\alpha(t)\}$ such that the Master Equation of ρ_t is of a form

$$\frac{d\rho_t}{dt} = L_t(\rho_t) = -i[H_t, \rho_t] + \sum_\alpha \left(X_\alpha(t)\rho_t X_\alpha(t)^* - \frac{1}{2}\{X_\alpha(t)^* X_\alpha(t), \rho_t\} \right),$$

for $\{A, B\} = AB + BA$ being the *anticommutator* of matrices A, B.

Proof. We will prove this theorem only partially, i.e. we will show the "if" part. The proof will be purely computational. Let us assume that the evolution Λ_t is differentiable and CP-divisible. This means, that – by putting ρ_t in a form $\rho_t = \Lambda_t(\rho_0)$ – we have,

$$\frac{d\rho_t}{dt} = \lim_{h\to 0^+} \frac{\rho_{t+h} - \rho_t}{h} = \lim_{h\to 0^+} \frac{\Lambda_{t+h}(\rho_0) - \Lambda_t(\rho_0)}{h},$$

where the derivative $\frac{d}{dt}$ is to be understood, by results of Section 1.3.2, in such way that we simply differentiate all matrix elements of ρ_t. The notation $h \to 0^+$ means taking the limit "from above", i.e. we assume $h \geq 0$; the resulting derivative will then be the "upper derivative". Now, using the divisibility of Λ_t we put $\Lambda_{t+h} = V_{t+h,t}\Lambda_t$ and write

$$\frac{d\rho_t}{dt} = \lim_{h\to 0^+} \frac{\Lambda_{t+h}(\rho_0) - \Lambda_t(\rho_0)}{h} = \lim_{h\to 0^+} \frac{V_{t+h,t}\Lambda_t(\rho_0) - \Lambda_t(\rho_0)}{h} = \lim_{h\to 0^+} \left(\frac{V_{t+h,t} - \mathrm{id}}{h} \right)(\rho_t),$$

so we have to effectively compute the derivative of an operator-valued function $x \mapsto V_{x,t}$ in $x = t$. Here we will make use of the complete positivity of propagator $V_{t,s}$. Namely, we can always put $V_{t,s}$ in a Kraus form (compare with Section 4.2), i.e. we can write

[11] The Reader may check that indeed differentiability of Λ_t implies its divisibility. The backwards implication is, however, false in general.

$$V_{t,s}(\rho) = \sum_{i=1}^{d} W_i(t,s)\rho W_i(t,s)^*$$

for some family $\{W_i(t,s) : s \leq t\}$ of two-parameter matrices of size d. So, returning to our main computation, we have to find, for arbitrarily chosen $\rho \in M_d(\mathbb{C})$,

$$\lim_{h\to 0^+} \frac{V_{t+h,t}(\rho) - \rho}{h} = \lim_{h\to 0^+} \frac{1}{h}\left(\sum_{i=1}^{d} W_i(t+h,t)\rho W_i(t+h,t)^* - \rho \right).$$

Since matrices $W_i(t,s)$ may be nonunique, we have to represent map $V_{t,s}$ in some clever way. Recall that in Section 2.1.1 we introduced a notion of a Hilbert-Schmidt orthonormal basis $\{F_i\}$, which spanned $M_d(\mathbb{C})$ as a (Hilbert) vector space. Such matrices could always be chosen in a way, that

$$F_i = F_i^*, \qquad F_{d^2} = \frac{1}{\sqrt{d}} I, \qquad \operatorname{tr} F_i F_j = \delta_{ij}, \qquad \operatorname{tr} F_i = \delta_{id^2}.$$

We can, therefore, expand matrices $W_i(t,s)$ in such a basis in order to obtain

$$W_i(t,s) = \sum_{j=1}^{d^2} w_{i,j}(t,s) F_j$$

for some complex coefficients $w_{i,j}(t,s)$. This allows to write

$$\sum_i W_i(t,s)\rho W_i(t,s)^* = \sum_i \sum_{j,k=1}^{d^2} w_{i,j}(t,s)\overline{w_{\imath,k}(t,s)} F_j \rho F_k^*.$$

Although we assumed the Hilbert-Schmidt basis to be Hermitian, we will keep the Hermitian adjoint notation F_k^* since it simplifies the calculations a little bit. Now, we can change the order of the summation,

$$\sum_i W_i(t,s)\rho W_i(t,s)^* = \sum_{j,k=1}^{d^2} \left(\sum_i w_{i,j}(t,s)\overline{w_{\imath,k}(t,s)} \right) F_j \rho F_k^*$$

and introduce a new matrix $[c_{jk}(t,s)]$ of size d^2, defined as

$$c_{jk}(t,s) = \sum_i w_{i,j}(t,s)\overline{w_{\imath,k}(t,s)}.$$

We encourage the Reader to verify that the matrix $[c_{jk}(t,s)]$ is positive semidefinite for all t,s. In result, we recast map $V_{t,s}$ into a form[12]

$$V_{t,s}(\rho) = \sum_{j,k=1}^{d^2} c_{jk}(t,s) F_j \rho F_k^*,$$

where all the time dependence is contained in a matrix of coefficients $[c_{jk}(t,s)]$. We substitute it back to the limiting procedure,

$$\lim_{h\to 0^+} \frac{V_{t+h,t}(\rho) - \rho}{h} = \lim_{h\to 0^+} \frac{1}{h}\left(\sum_{j,k=1}^{d^2} c_{jk}(t+h,t) F_j \rho F_k^* - \rho \right).$$

[12] In fact, we have essentially shown that every completely positive map on algebra $M_d(\mathbb{C})$ possesses such a form for some positive semidefinite matrix $[c_{jk}]$.

Now, we split the double sum into four distinct elements (we omit time parameters for brevity):

$$\sum_{j,k=1}^{d^2} c_{jk} F_j \rho F_k^* = \frac{1}{d} c_{d^2 d^2} \rho + \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} c_{j d^2} F_j \rho + \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} c_{d^2 j} \rho F_j^* + \sum_{j,k=1}^{d^2-1} c_{jk} F_j \rho F_k^*,$$

where we employed $F_{d^2} = \frac{1}{\sqrt{d}} I$. Let us introduce a matrix

$$Y_{t,s} = \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} c_{j d^2}(t,s) F_j.$$

Since matrix $[c_{jk}(t,s)]$ is positive semidefinite, it is also Hermitian, so $\overline{c_{jk}(t,s)} = c_{kj}(t,s)$. This means that $c_{d^2 j}(t,s) = \overline{c_{j d^2}(t,s)}$ and

$$\frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} c_{d^2 j}(t,s) \rho F_j^* = \rho \left(\frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} c_{j d^2}(t,s) F_j \right)^* = \rho Y_{t,s}^*.$$

This allows to write

$$\sum_{j,k=1}^{d^2} c_{jk}(t,s) F_j \rho F_k^* = \frac{1}{d} c_{d^2 d^2}(t,s) \rho + Y_{t,s} \rho + \rho Y_{t,s}^* + \sum_{j,k=1}^{d^2-1} c_{jk}(t,s) F_j \rho F_k^*,$$

which, after inserting back to our main calculation, yields

$$\lim_{h \to 0^+} \frac{V_{t+h,t}(\rho) - \rho}{h} = \lim_{h \to 0^+} \frac{1}{h} \left(z(t+h,t) \rho + Y_{t+h,t} \rho + \rho Y_{t+h,t}^* + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t) F_j \rho F_k^* \right),$$

where $z(t+h,t) = \frac{1}{d} [c_{d^2 d^2}(t+h,t) - 1]$. We now employ a second, important property of dynamical maps, namely the trace preservation. Recall, that $V_{t,s}$, being CP-divisible, was in particular demanded to be trace preserving, which means that for every $\rho \in M_d(\mathbb{C})$ we have $\operatorname{tr} V_{t,s}(\rho) = \operatorname{tr} \rho$. What does it mean in terms of the time derivative? Well, it is enough to compute

$$\operatorname{tr}[V_{t+h,t}(\rho) - \rho] = \operatorname{tr} V_{t+h,t}(\rho) - \operatorname{tr} \rho = 0,$$

where we used linearity of trace. We therefore have, that the whole expression under the limit must be of zero trace. Let us put all of it in slightly different form. For this, we define two new matrices

$$A_{t,h} = \frac{1}{2} \left(Y_{t+h,t} + Y_{t+h,t}^* \right), \qquad B_{t,h} = \frac{1}{2i} \left(Y_{t+h,t} - Y_{t+h,t}^* \right),$$

which together constitute for so-called Cartesian decomposition of matrix $Y_{t+h,t}$, i.e.

$$Y_{t+h,t} = A_{t,h} + i B_{t,h}.$$

The Reader may check that both $A_{t,h}$ and $B_{t,h}$ are, by construction, Hermitian; this allows to simply put $Y_{t+h,t}^* = A_{t,h} - i B_{t,h}$ and then, the expression under the limit transforms into

$$\begin{aligned} & z(t+h,t) \rho + Y_{t+h,t} \rho + \rho Y_{t+h,t}^* + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t) F_j \rho F_k^* \\ & = z(t+h,t) \rho + \left(A_{t,h} + i B_{t,h} \right) \rho + \rho \left(A_{t,h} - i B_{t,h} \right) + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t) F_j \rho F_k^* \end{aligned}$$

$$= z(t+h,t)\rho + A_{t,h}\rho + \rho A_{t,h} + i\big(B_{t,h}\rho - \rho B_{t,h}\big) + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_j\rho F_k^*$$

$$= z(t+h,t)\rho + \{A_{t,h},\rho\} + i[B_{t,h},\rho] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_j\rho F_k^*.$$

Notice, that the first term is of a form

$$z(t+h,t)\rho = z(t+h,t)\left(\frac{1}{2}\rho I + \frac{1}{2}I\rho\right) = \frac{1}{2}z(t+h,t)\{I,\rho\},$$

which, after putting back and using linearity of the anticommutator, yields

$$\frac{1}{2}z(t+h,t)\{I,\rho\} + \{A_{t,h},\rho\} + i[B_{t,h},\rho] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_j\rho F_k^*$$

$$= \{C_{t,h},\rho\} + i[B_{t,h},\rho] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_j\rho F_k^*,$$

where $C_{t,h} = A_{t,h} + \frac{1}{2}z(t+h,t)I$. The trace of the above must vanish, so the Reader may check – using properties of a trace,

$$\operatorname{tr} AB = \operatorname{tr} BA\,, \qquad \operatorname{tr}[A,B] = 0, \qquad \operatorname{tr}\{A,B\} = 2\operatorname{tr} AB,$$

that this condition yields

$$0 = \operatorname{tr}\left[\{C_{t,h},\rho\} + i[B_{t,h},\rho] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_j\rho F_k^*\right]$$

$$= \operatorname{tr}\{C_{t,h},\rho\} + i\operatorname{tr}[B_{t,h},\rho] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)\operatorname{tr} F_j\rho F_k^*$$

$$= 2\operatorname{tr} C_{t,h}\rho + \operatorname{tr}\sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_k^*F_j\rho$$

$$= \operatorname{tr}\left(2C_{t,h} + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_k^*F_j\right)\rho.$$

Note, that the above must vanish *regardless of a choice of* ρ, but – because of linearity of trace – this is possible if and only if

$$2C_{t,h} + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_k^*F_j = 0,$$

or, if

$$C_{t,h} = -\frac{1}{2}\sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_k^*F_j.$$

We can now put this back into our expression with a limit,

$$\lim_{h\to 0^+}\frac{V_{t+h,t}(\rho)-\rho}{h} = \lim_{h\to 0^+}\frac{1}{h}\left(\{C_{t,h},\rho\} + i[B_{t,h},\rho] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t)F_j\rho F_k^*\right)$$

$$= \lim_{h\to 0^+} \frac{1}{h}\left(i\big[B_{t,h},\rho\big] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t) F_j \rho F_k^* - \frac{1}{2}\left\{ \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t) F_k^* F_j \,, \rho \right\} \right)$$
$$= \lim_{h\to 0^+} \frac{1}{h}\left(i\big[B_{t,h},\rho\big] + \sum_{j,k=1}^{d^2-1} c_{jk}(t+h,t) \left(F_j \rho F_k^* - \frac{1}{2}\{F_k^* F_j, \rho\} \right) \right).$$

Now we will revert all our substitutions and calculate the limit. Recall that

$$B_{t,h} = \frac{1}{2i}\big(Y_{t+h,t} - Y_{t+h,t}^*\big) = \frac{-i}{2\sqrt{d}} \left(\sum_{j=1}^{d^2-1} c_{jd^2}(t+h,t) F_j - \sum_{j=1}^{d^2-1} \overline{c_{jd^2}(t,s)} F_j^* \right),$$

so computing $\lim_{h\to 0^+} \frac{1}{h} B_{t,h}$ involves computing limits of a form $\lim_{h\to 0^+} \frac{1}{h} c_{jd^2}(t+h,t)$. Note, that functions $c_{jk}(t,s)$ were defined as coefficients in the Kraus-like decomposition of the propagator $V_{t,s}$. Since propagator is required to satisfy Chapman-Kolmogorov identities, we have $V_{t,t} = \mathrm{id}$, so

$$V_{t,t}(\rho) = \sum_{j,k=1}^{d^2} c_{jk}(t,t) F_j \rho F_k^* = \rho.$$

But the sum in the above expression can be equal to ρ if and only if just matrices $F_{d_2} = \frac{1}{\sqrt{d}} I$ remain, or if

$$V_{t,t}(\rho) = I\rho I = c_{d^2 d^2}(t,t)\sqrt{d} F_{d^2} \rho \sqrt{d} F_{d^2}^*,$$

which simply means, that

$$c_{jk}(t,t) = 0 \ \text{ if } j,k < d^2, \qquad c_{jd^2}(t,t) = 0 \quad \text{and} \quad c_{d^2 d^2}(t,t) = \frac{1}{d}.$$

This means, that

$$\lim_{h\to 0^+} \frac{1}{h} c_{jk}(t+h,t) = \lim_{h\to 0^+} \frac{c_{jk}(t+h,t) - c_{jk}(t,t)}{h} = \frac{\partial}{\partial \xi}\Big|_{\eta=\xi} c_{jk}(\xi,\eta), \qquad \text{for } j,k < d^2,$$

and analogously

$$\lim_{h\to 0^+} \frac{1}{h} c_{jd^2}(t+h,t) = \frac{\partial}{\partial \xi}\Big|_{\eta=\xi} c_{jd^2}(\xi,\eta).$$

The above calculation shows that the requested limits of expressions $\frac{1}{h} c_{jk}(t+h,t)$ appearing in the limiting procedure are simply *partial derivatives* of the coefficients $c_{jk}(t,s)$. However, our initial assumption on differentiability of the dynamics implies, that the propagator $V_{t,s}$ must be also differentiable with respect to both time variables (verify it!), which will be the case if and only if all functions $c_{jk}(t,s)$ appearing in the decomposition $V_{t,s} = \sum_{j,k=1}^{d^2} c_{jk}(t,s) F_j \rho F_k^*$ are differentiable. This means, that all limits of a form $\lim_{h\to 0^+} \frac{1}{h} c_{jd^2}(t+h,t)$ exists and can be expressed as some new functions of variable t. Let us then define a set of functions $\{t \mapsto \gamma_{jk}(t)\}$ by setting

$$\gamma_{jd^2}(t) = \lim_{h\to 0^+} \frac{1}{h} c_{jd^2}(t+h,t)\,, \qquad \gamma_{jk}(t) = \lim_{h\to 0^+} \frac{1}{h} c_{jk}(t+h,t).$$

This finally allows to execute the limiting procedure in order to obtain

$$\lim_{h\to 0^+} B_{t,h} = \frac{-i}{2\sqrt{d}} \left(\sum_{j=1}^{d^2-1} \gamma_{jd^2}(t) F_j - i \sum_{j=1}^{d^2-1} \overline{\gamma_{jd^2}(t)} F_j^* \right) = -H_t,$$

where we introduced a new time-dependent matrix H_t being, by direct check, still Hermitian. This, together with functions $\gamma_{jk}(t)$, finally yields

$$\lim_{h\to 0^+}\frac{V_{t+h,t}(\rho)-\rho}{h}=-i[H_t,\rho]+\sum_{j,k=1}^{d^2-1}\gamma_{jk}(t)\left(F_j\rho F_k^*-\frac{1}{2}\{F_k^*F_j,\rho\}\right).$$

We have therefore obtained a new time-dependent linear map defined on $M_d(\mathbb{C})$, which action on any $\rho\in M_d(\mathbb{C})$ is given via formula

$$L_t(\rho)=-i[H_t,\rho]+\sum_{j,k=1}^{d^2-1}\gamma_{jk}(t)\left(F_j\rho F_k^*-\frac{1}{2}\{F_k^*F_j,\rho\}\right)$$

for some Hermitian H_t and some complex-valued functions $\gamma_{jk}(t)$. This map is commonly called the **Lindblad-Gorini-Kossakowski-Sudarshan generator**, or simply the **Lindbladian** or **Liouvillean**. Now, remembering that the very beginning of this long calculation was devoted to finding the time derivative of a density matrix, we may finally put

$$\frac{d\rho_t}{dt}=\lim_{h\to 0^+}\frac{V_{t+h,t}(\rho_t)-\rho_t}{h}=L_t(\rho_t).$$

We see then, that the Lindbladian L_t determines the dynamics of density operator which evolution is Markovian (CP-divisible) and differentiable. It remains to be shown that L_t admits a form claimed in the theorem. For this we first notice that the matrix $[\gamma_{jk}(t)]$ of size d^2, the so-called **Kossakowski matrix**, is in fact positive semidefinite. To see this, take any complex vector $\xi\in\mathbb{C}^{d^2}$ and simply calculate

$$\begin{aligned}\langle\xi,[\gamma_{jk}(t)]\xi\rangle&=\sum_{j,k=1}^{d^2}\gamma_{jk}(t)\bar{\xi}_j\xi_k=\sum_{j,k=1}^{d^2}\left(\lim_{h\to 0^+}\frac{1}{h}c_{jk}(t+h,t)\right)\bar{\xi}_j\xi_k\\&=\lim_{h\to 0^+}\frac{1}{h}\sum_{j,k=1}^{d^2}c_{jk}(t+h,t)\bar{\xi}_j\xi_k=\lim_{h\to 0^+}\frac{1}{h}g_\xi(t+h),\end{aligned}$$

where $g_\xi(t+h)=\sum_{j,k=1}^{d^2}c_{jk}(t+h,t)\bar{\xi}_j\xi_k$. Now, recall that in order for $V_{t,s}$ being completely positive, the matrix $[c_{jk}(t,s)]$ had to be positive semidefinite. This means, that function g_ξ must have nonnegative values and the limit $\lim_{h\to 0^+}\frac{1}{h}g_\xi(t+h)$ is also nonnegative for every t, i.e. Kossakowski matrix is positive semidefinite for all t. From Section 2.2 we know, that if a matrix A is positive semidefinite, then it may be expressed as

$$A=B^*B$$

for some other matrix B. This then means, that there exists some matrix $[w_{jk}(t)]\in M_{d^2}(\mathbb{C})$ such, that

$$[\gamma_{jk}(t)]=[w_{jk}(t)]^*[w_{jk}(t)],$$

or, more explicitly,

$$\gamma_{jk}(t)=\sum_{\alpha=1}^{d^2}\overline{w_{\alpha j}(t)}w_{\alpha k}(t).$$

If we put this into our expression for L_t we obtain

$$L_t(\rho)=-i[H_t,\rho]+\sum_{j,k=1}^{d^2-1}\sum_{\alpha=1}^{d^2}\overline{w_{\alpha j}(t)}w_{\alpha k}(t)\left(F_j\rho F_k^*-\frac{1}{2}\{F_k^*F_j,\rho\}\right)$$

$$= -i[H_t, \rho] + \sum_{\alpha=1}^{d^2} \left(\sum_{j=1}^{d^2-1} \overline{w_{\alpha J}(t)} F_j \cdot \rho \cdot \sum_{k=1}^{d^2-1} w_{\alpha k}(t) F_k^* - \frac{1}{2} \left\{ \sum_{k=1}^{d^2-1} w_{\alpha k}(t) F_k^* \cdot \sum_{j=1}^{d^2-1} \overline{w_{\alpha J}(t)} F_j , \rho \right\} \right)$$
$$= -i[H_t, \rho] + \sum_{\alpha=1}^{d^2} \left(X_\alpha(t) \rho X_\alpha(t)^* - \frac{1}{2} \{ X_\alpha(t)^* X_\alpha(t), \rho \} \right),$$

where we introduced a new set of matrices

$$X_\alpha(t) = \sum_{j=1}^{d^2-1} \overline{w_{\alpha J}(t)} F_j.$$

So, this is it. We have shown, that indeed, any Markovian differentiable quantum dynamical map satisfies the Markovian Master Equation determined by Lindbladian L_t of a claimed form, which is sometimes referred to as the **LGKS form** or simply **the standard form**. This is the end of the proof of the "if" direction of the theorem. The remaining "only if" direction may be found by inquisitive Readers in numerous sources, for example in [3]. □

We have then derived an exact, explicit form of the Markovian Master Equation

$$\frac{d\rho_t}{dt} = L_t(\rho_t)$$

for L_t is a standard form given in two equivalent forms as

$$L_t(\rho) = -i[H_t, \rho] + \sum_{j,k=1}^{d^2-1} \gamma_{jk}(t) \left(F_j \rho F_k^* - \frac{1}{2} \{ F_k^* F_j, \rho \} \right)$$
$$= -i[H_t, \rho] + \sum_{\alpha=1}^{d^2} \left(X_\alpha(t) \rho X_\alpha(t)^* - \frac{1}{2} \{ X_\alpha(t)^* X_\alpha(t), \rho \} \right).$$

If we recast this equation into a little more convenient form

$$\frac{d\rho_t}{dt} = -i[H_t, \rho_t] + D_t(\rho_t)$$

for map D_t to be easily deciphered to involve all the terms with a Kossakowski matrix, called the **dissipator** sometimes, it is immediate and straightforward to note that Master Equation is a direct generalization of the *von Neumann equation* for density matrix,

$$\frac{d\rho_t}{dt} = -i[H_t, \rho_t].$$

The formal difference between these two equations is naturally the presence of a dissipator D_t, which was totally absent in von Neumann equation. If we recall, that we constructed the Master Equation under assumption that *the system of interest was open*, i.e. was allowed to interact with its environment in a way, which generated a completely positive and trace preserving evolution, then it is clear that matrix H_t appearing in the Lindbladian can be interpreted as a Hamiltonian[13], and the appearance of dissipator D_t is due to the influence on the system from the environment, i.e. it expresses results of the interaction.

[13] We make a technical note here, that although H_t indeed bears an interpretation of the Hamiltonian, one can show that in general it will be different from the **free** Hamiltonian of a system, since it contains some perturbations (*Lamb shifts*) due to the interaction with the environment.

Now, we make yet another remark. Remember, that $\rho_t = \Lambda_t(\rho_0)$ for ρ_0 being the density matrix in the initial time $t = 0$. Substituting this back into the Master Equation, we have

$$\frac{d\rho_t}{dt} = \frac{d}{dt}\Lambda_t(\rho_0) = \frac{d\Lambda_t}{dt}(\rho_0) = L_t\Lambda_t(\rho_0),$$

so in fact, the very quantum dynamical map Λ_t satisfies its own, operator version of the Master Equation,

$$\frac{d\Lambda_t}{dt} = L_t\Lambda_t.$$

Our analysis was invoked on the matrix space $M_d(\mathbb{C})$. This is finite dimensional vector space, which is isomorphic to space $\mathbb{C}^{d^2}$. The Master Equation is therefore an ordinary differential equation defined on vector functions with values in $\mathbb{C}^{d^2}$. This means, that the action of any linear map on matrices from $M_d(\mathbb{C})$ is completely equivalent to the action of some linear operator on space $\mathbb{C}^{d^2}$. This however can always be represented as some square matrix of size d^2. This means, that one can – by employing one of so-called *vectorization* schemes – treat every matrix $A \in M_d(\mathbb{C})$ as a complex vector $\mathbf{a} \in \mathbb{C}^{d^2}$ and every map T on matrix space $M_d(\mathbb{C})$ may be treated as a matrix $\mathbf{T} = [t_{ij}] \in M_{d^2}(\mathbb{C})$. Then, action $T(A)$ can be isomorphically represented as $\mathbf{Ta}$, a multiplication of matrix and a vector. And so, if one represents a density matrix ρ_t as some complex vector $\mathbf{r}_t \in \mathbb{C}^{d^2}$ and maps L_t and Λ_t as some matrices $\mathbf{L}_t, \mathbf{\Lambda}_t \in M_{d^2}(\mathbb{C})$, then it is straightforward to see, that the Master Equation transforms into form

$$\frac{d\mathbf{r}_t}{dt} = \mathbf{L}_t\mathbf{r}_t, \qquad \text{or, equivalently} \qquad \frac{d\mathbf{\Lambda}_t}{dt} = \mathbf{L}_t\mathbf{\Lambda}_t.$$

This matrix form of Master Equation simply suggests that matrix $\mathbf{\Lambda}_t$ is simply a **fundamental matrix solution** of the Master Equation, and, since $\Lambda_0 = \mathrm{id}$ and therefore $\mathbf{\Lambda}_0 = I$, even **principal**. However, since such a "vectorized" picture is completely equivalent to the original one, we make no distinction between these two and so we can call directly Λ_t a *principal matrix solution*, abusing the terminology a little bit.

7.3. Quantum Dynamical Semigroups

Unfortunately, despite its mathematical elegance and closed form, the Master Equation given as previously can be difficult to be solved analytically, which is due to general time dependence of the generator L_t. There are no known algorithms for obtaining solutions of such equations in case a general dependence $t \mapsto L_t$, apart from some very formal approaches, involving asymptotic expressions or recurrent integration and series expansions[14]. Closed form expressions for Λ_t may be found in very few cases. One of them is the case of a constant Lindbladian. Namely, if we assume that $L_t = L$ is time independent (i.e., both the Hamiltonian and the dissipator are constant), we end up with an autonomous Master Equation

$$\frac{d\rho_t}{dt} = L(\rho_t).$$

Again, switching to the "vectorized" picture sketched above, one immediately sees that the principal fundamental solution of such equation will be, according to Section 1.3.4, given in terms of the exponential

$$\Lambda_t = e^{tL},$$

where the exponentiation is to be again understood in terms of a power series (compare with Section 1.3.4),

[14] These include the time-splitting formula, time-ordered exponentials and Dyson, Magnus or Fer expansions.

$$e^{tL} = \sum_{n=0}^{\infty} \frac{t^n L^n}{n!}.$$

It is also very easy to see that a quantum dynamical map given by such expression, i.e. a family of linear maps $\{e^{tL} : t \geq 0\}$, is a *semigroup* (a *monoid*, to be precise – see Section 1.1.1), known as a celebrated *Quantum Dynamical Semigroup*:

Definition 25. A family $\{e^{tL} : t \geq 0\}$ of completely positive and trace preserving maps on *-algebra $M_d(\mathbb{C})$, where L is a (constant) Lindbladian in standard form,

$$L(\rho) = -i[H, \rho] + \sum_{\alpha} \left(X_\alpha \rho X_\alpha^* - \frac{1}{2}\{X_\alpha^* X_\alpha, \rho\} \right)$$

for some Hermitian matrix H and finite family of matrices $\{X_\alpha\}$, is a semigroup called the *Quantum Dynamical Semigroup*.

8. Microscopic derivation and weak coupling limit

This section will be devoted to establishing a link between mathematical structure of completely positive quantum evolution and its underlying principles of purely physical nature. We recall that our microscopic model of open quantum system S was characterized by system's self Hamiltonian H (for simplicity we assume all Hamiltonians to be time independent) and Hilbert space $\mathcal{H} \simeq \mathbb{C}^d$, while the reservoir E was described by Hamiltonian H_E and Hilbert space $\mathcal{H}_E$. The interaction between systems S and E was encoded in an interaction Hamiltonian H_{int} of a form

$$H_{\text{int}} = \sum_{\alpha} S_\alpha \otimes R_\alpha,$$

where $S_\alpha \in M_d(\mathbb{C})$ and $R_\alpha \in B(\mathcal{H}_E)$ were interpreted as operators acting on system's and reservoir's part of a joint Hilbert space $\mathcal{H}_{SE} = \mathcal{H}_S \otimes \mathcal{H}_E$. We will eventually invoke the so-called *weak coupling limit approximation*, in which we explicitly assume the interaction to be weak in a sense, so the reservoir is not perturbed by internal changes occurring in the system S.

We will now derive the Markovian Master Equation solely from this underlying Hamiltonian model and without assuming complete positivity a priori. First, remember that we have already remarked on the fact, that the entire system $S + E$ can be pretty much assumed to be isolated. As such, the evolution of the joint density operator σ_t of system $S + E$ must be given by von Neumann equation, as we already elaborated in Section 6.1,

$$\frac{d\sigma_t}{dt} = -i[H_{SE}, \sigma_t].$$

with a solution

$$\sigma_t = e^{-iH_{SE}t} \sigma_0 e^{iH_{SE}t}.$$

We are interested only in the evolution of the subsystem S, since the environment is way too huge for us to describe, or even to measure thoroughly. This means, that we have to average the joint density operator σ_t with respect to degrees of freedom of subsystem E, or, to compute the partial trace of σ_t over Hilbert space $\mathcal{H}_E$. This brings us the expression for reduced density matrix of subsystem S,

$$\rho_t = \text{tr}_E\, \sigma_t = \text{tr}_E\, e^{-iH_{SE}t} \tilde{\rho}_0 e^{iH_{SE}t}.$$

Now we will employ, purely for convenience, a standard mathematical "trick" of switching to the so-called *interaction picture*. Namely, we define a following transformation

$$A \mapsto \tilde{A}(t) = e^{iH_{SE}^0 t} A e^{-iH_{SE}^0 t},$$

where $H_{SE}^0 = H_{SE} - H_{\mathrm{int}}$ is the "free" part of the joint Hamiltonian (missing the interaction term). In this manner we define the interaction picture counterpart of the density operator

$$\tilde{\sigma}_t = e^{iH_{SE}^0 t}\sigma_t e^{-iH_{SE}^0 t}.$$

The purpose of such transformation is to simplify the differential equation we have to solve. Namely, when we compute the time derivative of such transformed density operator, we get

$$\begin{aligned}
\frac{d\tilde{\sigma}_t}{dt} &= \frac{d}{dt}e^{iH_{SE}^0 t}\sigma_t e^{-iH_{SE}^0 t} \\
&= \left(\frac{d}{dt}e^{iH_{SE}^0 t}\right)\sigma_t e^{-iH_{SE}^0 t} + e^{iH_{SE}^0 t}\frac{d\sigma_t}{dt}e^{-iH_{SE}^0 t} + e^{iH_{SE}^0 t}\sigma_t\left(\frac{d}{dt}e^{-iH_{SE}^0 t}\right) \\
&= iH_{SE}^0 e^{iH_{SE}^0 t}\sigma_t e^{-iH_{SE}^0 t} - ie^{iH_{SE}^0 t}[H_{SE},\sigma_t]e^{-iH_{SE}^0 t} - ie^{iH_{SE}^0 t}\sigma_t e^{-iH_{SE}^0 t}H_{SE}^0 \\
&= iH_{SE}^0\tilde{\sigma}_t - ie^{iH_{SE}^0 t}[H_{SE},\sigma_t]e^{-iH_{SE}^0 t} - i\tilde{\sigma}_t H_{SE}^0 \\
&= i[H_{SE}^0,\tilde{\sigma}_t] - ie^{iH_{SE}^0 t}(H_{SE}\sigma_t - \sigma_t H_{SE})e^{-iH_{SE}^0 t} \\
&= i[H_{SE}^0,\tilde{\sigma}_t] - i\left(e^{iH_{SE}^0 t}H_{SE}e^{-iH_{SE}^0 t}e^{iH_{SE}^0 t}\sigma_t e^{-iH_{SE}^0 t} - e^{iH_{SE}^0 t}\sigma_t e^{-iH_{SE}^0 t}e^{iH_{SE}^0 t}H_{SE}e^{-iH_{SE}^0 t}\right) \\
&= i[H_{SE}^0,\tilde{\sigma}_t] - i\left(\tilde{H}_{SE}(t)\tilde{\sigma}_t - \tilde{\sigma}_t\tilde{H}_{SE}(t)\right) = i[H_{SE}^0,\tilde{\sigma}_t] - i\big[\tilde{H}_{SE}(t),\tilde{\sigma}_t\big] = i\big[H_{SE}^0 - \tilde{H}_{SE}(t),\tilde{\sigma}_t\big] \\
&= i\left[e^{iH_{SE}^0 t}H_{SE}^0 e^{-iH_{SE}^0 t} - e^{iH_{SE}^0 t}H_{SE}e^{-iH_{SE}^0 t},\tilde{\sigma}_t\right] \\
&= i\left[e^{iH_{SE}^0 t}(H_{SE}^0 - H_{SE})e^{-iH_{SE}^0 t},\tilde{\sigma}_t\right] = i\left[e^{iH_{SE}^0 t}(H_{SE} - H_{\mathrm{int}} - H_{SE})e^{-iH_{SE}^0 t},\tilde{\sigma}_t\right] \\
&= -i\left[e^{iH_{SE}^0 t}H_{\mathrm{int}}e^{-iH_{SE}^0 t},\tilde{\sigma}_t\right] = -i\big[\tilde{H}_{\mathrm{int}}(t),\tilde{\sigma}_t\big],
\end{aligned}$$

so in the interaction picture the only term which remains is the interaction one, however now explicitly time-dependent,

$$\frac{d\tilde{\sigma}_t}{dt} = -i\big[\tilde{H}_{\mathrm{int}}(t),\tilde{\sigma}_t\big], \qquad \tilde{H}_{\mathrm{int}}(t) = e^{iH_{SE}^0 t}H_{\mathrm{int}}e^{-iH_{SE}^0 t} = \sum_\alpha \tilde{S}_\alpha(t)\otimes\tilde{R}_\alpha(t),$$

for operators $\tilde{S}_\alpha(t)$ and $\tilde{R}_\alpha(t)$ being then the interaction picture counterparts of S_α and R_α,

$$\tilde{S}_\alpha(t) = e^{iHt}S_\alpha e^{-iHt}, \qquad R_\alpha(t) = e^{iH_E t}R_\alpha e^{-iH_E t}.$$

Let us now *solve* this equation, at least formally. We know the derivative of $\tilde{\sigma}_t$, so obtaining the actual function $t \mapsto \tilde{\sigma}_t$ involves only integrating both sides of the ODE:

$$\tilde{\sigma}_t - \tilde{\sigma}_0 = \int_0^t \frac{d\tilde{\sigma}_{t'}}{dt'}dt' = -i\int_0^t \big[\tilde{H}_{\mathrm{int}}(t'),\tilde{\sigma}_{t'}\big]dt',$$

which naturally has no apparent use for us, since the unknown function now appears at both sides of the resulting integral equation,

$$\tilde{\sigma}_t = \tilde{\sigma}_0 - i\int_0^t \big[\tilde{H}_{\mathrm{int}}(t'),\tilde{\sigma}_{t'}\big]dt',$$

and we have not actually proceeded any step towards obtaining the actual solution. In fact, we can complexify the situation even a little but more by replacing $\tilde{\sigma}_{t'}$ under the integral by the whole expression again,

$$\tilde{\sigma}_t = \tilde{\sigma}_0 - i\int_0^t \big[\tilde{H}_{\mathrm{int}}(t'),\tilde{\sigma}_{t'}\big]dt'$$

$$= \tilde{\sigma}_0 - i\int_0^t \left[\tilde{H}_{\mathrm{int}}(t'), \tilde{\sigma}_0 - i\int_0^{t'} \left[\tilde{H}_{\mathrm{int}}(t''), \tilde{\sigma}_{t''}\right] dt''\right] dt'$$
$$= \tilde{\sigma}_0 - i\int_0^t \left[\tilde{H}_{\mathrm{int}}(t'), \tilde{\sigma}_0\right] dt' - \int_0^t \int_0^{t'} \left[\tilde{H}_{\mathrm{int}}(t'), \left[\tilde{H}_{\mathrm{int}}(t''), \tilde{\sigma}_{t''}\right]\right] dt''\, dt',$$

or, by differentiating,

$$\frac{d\tilde{\sigma}_t}{dt} = -i\left[\tilde{H}_{\mathrm{int}}(t), \tilde{\sigma}_0\right] - \int_0^t \left[\tilde{H}_{\mathrm{int}}(t), \left[\tilde{H}_{\mathrm{int}}(t'), \tilde{\sigma}_{t'}\right]\right] dt'.$$

Let us now return to the reduced density matrix, which will now be also in the interaction picture, $\tilde{\rho}_t = \mathrm{tr}_E\, \tilde{\sigma}_t$. Its dynamics will be now governed by the patrial trace of the above, i.e.

$$\frac{d\tilde{\rho}_t}{dt} = \frac{d}{dt}\mathrm{tr}_E\, \tilde{\sigma}_t = -i\,\mathrm{tr}_E\left[\tilde{H}_{\mathrm{int}}(t), \tilde{\sigma}_0\right] - \int_0^t \mathrm{tr}_E\left[\tilde{H}_{\mathrm{int}}(t), \left[\tilde{H}_{\mathrm{int}}(t'), \tilde{\sigma}_{t'}\right]\right] dt'.$$

We now make a crucial assumption here, called the Born approximation. Namely, we say that the coupling between systems S and E is so weak, that the environment is not perturbed by the interaction in any significant way, or that the excitations in the environment due to the interaction with system S decay so rapidly that E effectively remains in its equilibrium state, i.e.

$$\tilde{\sigma}_t = \tilde{\rho}_t \otimes \rho_E,$$

where ρ_E is a **constant** state of E. If, however, it is constant, it must commute with environment's Hamiltonian H_E, which implies that the interaction picture of ρ_E is simply ρ_E (without time dependence). Now, the first term at the right hand side of our expression for $\frac{d\tilde{\rho}_t}{dt}$ can be computed to be (show it!)

$$-i\,\mathrm{tr}_E\left[\tilde{H}_{\mathrm{int}}(t), \tilde{\sigma}_0\right] = -i\sum_\alpha \left[\tilde{S}_\alpha(t), \rho_0\right] \mathrm{tr}_E\, R_\alpha \rho_E$$

where we employed the decomposition of the interaction Hamiltonian in interaction picture. Expressions $\mathrm{tr}_E\, R_\alpha \rho_E$ are then simply the expectation values of operators R_α computed in the environmental equilibrium state. One can show that we can always define the energy scale of the system in such a way, that those expectation values can be assumed to be 0, which is a great simplification; this, together with a Born approximation, leads to

$$\frac{d\tilde{\rho}_t}{dt} = -\int_0^t \mathrm{tr}_E\left[\tilde{H}_{\mathrm{int}}(t), \left[\tilde{H}_{\mathrm{int}}(t'), \tilde{\rho}_{t'} \otimes \rho_E\right]\right] dt'.$$

Notice, that we have two time variables at the right hand side, t and t'; from the construction of the integral it is clear that necessarily $t' \leq t$. This means, that the rate of change of $\tilde{\rho}_t$ depend on values of $\tilde{\rho}_{t'}$, i.e. the **history** of the state. Therefore, it is time for invoking the celebrated *Markovian approximation* where we explicitly delete this time dependence, i.e. we replace $\tilde{\rho}_{t'}$ with $\tilde{\rho}_t$,

$$\frac{d\tilde{\rho}_t}{dt} = -\int_0^t \mathrm{tr}_E\left[\tilde{H}_{\mathrm{int}}(t), \left[\tilde{H}_{\mathrm{int}}(t'), \tilde{\rho}_t \otimes \rho_E\right]\right] dt',$$

obtaining the so-called *Redfield equation*. Now, in order to proceed one shows, using quite a demanding mathematical apparatus which lays way beyond the scope of this lecture, that we can rewrite this equation into a form

$$\frac{d\tilde{\rho}_t}{dt} = -\int_0^\infty \mathrm{tr}_E \left[\tilde{H}_{\mathrm{int}}(t), \left[\tilde{H}_{\mathrm{int}}(t-t'), \tilde{\rho}_t \otimes \rho_E\right]\right] dt',$$

which can be justified if the integrand disappears sufficiently fast, which is the case here since we assume that the characteristic time after which internal correlation in the environment decay, is very short. This final – however the most demanding – trick finally leaves us with the proper Markovian Master Equation, which we now reshape a little bit.

First, one can show that operators $\tilde{S}_\alpha(t)$ appearing in the interaction picture Hamiltonian can be decomposed into sums

$$\tilde{S}_\alpha(t) = \sum_\omega S_\alpha(\omega) e^{i\omega t},$$

where numbers ω are defined as differences between eigenvalues of system's Hamiltonian H, called *Bohr frequencies*. This allows to rework the double commutator,

$$\begin{aligned}\frac{d\tilde{\rho}_t}{dt} &= -\sum_{\alpha,\beta}\int_0^\infty \mathrm{tr}_E \left[\tilde{S}_\alpha(t)\otimes\tilde{R}_\alpha(t), \left[\tilde{S}_\beta(t-t')\otimes\tilde{R}_\beta(t-t'), \tilde{\rho}_t\otimes\rho_E\right]\right] dt' \\ &= \sum_{\omega,\omega'}\sum_{\alpha,\beta} e^{i(\omega-\omega')t}\Gamma_{\alpha\beta}(\omega)\left(S_\beta(\omega)\tilde{\rho}_t S_\alpha(\omega')^* - S_\alpha(\omega')^* S_\beta(\omega)\tilde{\rho}_t\right) + \mathrm{h.c.}\end{aligned}$$

which can be checked by the Reader with a bit of algebraic work., where we introduced the so-called *one-sided Fourier transforms*

$$\Gamma_{\alpha\beta}(\omega) = \int_0^\infty e^{i\omega t'}\,\mathrm{tr}_E\, R_\alpha(t)^* R_\beta(t-t')\,dt'.$$

Functions in the integrand, $a_{\alpha\beta}(t,t') = \mathrm{tr}_E\, R_\alpha(t)^* R_\beta(t-t')$, are commonly called the *reservoir autocorrelation functions*. Second, we employ the **rotating wave approximation**: we neglect all terms proportional to $e^{i(\omega-\omega')t}$ for $\omega \neq \omega'$ since they "rotate" very quickly and therefore their averaged contribution is effectively negligible; this yields

$$\frac{d\tilde{\rho}_t}{dt} = \sum_\omega\sum_{\alpha,\beta}\Gamma_{\alpha\beta}(\omega)\left(S_\beta(\omega)\tilde{\rho}_t S_\alpha(\omega)^* - S_\alpha(\omega)^* S_\beta(\omega)\tilde{\rho}_t\right) + \mathrm{h.c.}$$

Third, we compute a Cartesian decomposition of a matrix $\left[\Gamma_{\alpha\beta}(\omega)\right]_{\alpha\beta}$, i.e. we introduce two Hermitian matrices

$$\left[\gamma_{\alpha\beta}(\omega)\right] = \left[\Gamma_{\alpha\beta}(\omega)\right] + \left[\Gamma_{\alpha\beta}(\omega)\right]^*, \qquad \left[s_{\alpha\beta}(\omega)\right] = \frac{1}{2i}\left(\left[\Gamma_{\alpha\beta}(\omega)\right] - \left[\Gamma_{\alpha\beta}(\omega)\right]^*\right)$$

such that $\left[\Gamma_{\alpha\beta}(\omega)\right] = \frac{1}{2}\left[\gamma_{\alpha\beta}(\omega)\right] + i\left[s_{\alpha\beta}(\omega)\right]$ (we put $\frac{1}{2}$ for convenience). Such decomposition now allows to recast our equation into a form (check it!)

$$\frac{d\tilde{\rho}_t}{dt} = -i[\Delta,\tilde{\rho}_t] + \sum_\omega\sum_{\alpha,\beta}\gamma_{\alpha\beta}(\omega)\left(S_\beta(\omega)\tilde{\rho}_t S_\alpha(\omega)^* - \frac{1}{2}\left\{S_\alpha(\omega)^* S_\beta(\omega), \tilde{\rho}_t\right\}\right),$$

where Δ is a Hermitian matrix defined as

$$\Delta = \sum_\omega\sum_{\alpha,\beta} s_{\alpha\beta}(\omega) S_\alpha(\omega)^* S_\beta(\omega).$$

Now, it remains only to revert back to the original Schrödinger picture, which we leave to the Reader as an exercise. After all the tedious work we have done so far, we end up with a following equation in Schrodinger picture,

$$\frac{d\rho_t}{dt} = -i[H + \Delta, \rho_t] + \sum_{\omega} \sum_{\alpha,\beta} \gamma_{\alpha\beta}(\omega) \left(S_\beta(\omega) \tilde{\rho}_t S_\alpha(\omega)^* - \frac{1}{2} \{ S_\alpha(\omega)^* S_\beta(\omega), \tilde{\rho}_t \} \right),$$

and what remains to be shown, in order to identify the above as the autonomous Markovian Master Equation, is positive semidefiniteness of matrix $[\gamma_{\alpha\beta}(\omega)]$ for each ω. This however may be found in literature [1] [4] to be indeed true; we will not however dive into details here. To summarize everything up, we have indeed obtained the Markovian Master Equation given in terms of a time-independent generator of Lindblad-Gorini-Kossakowski-Sudarshan form. The term Δ, which is being added to the system's free Hamiltonian, is called the *Lamb shift Hamiltonian* and it effectively shifts energy levels of the system (sometimes of considerable amounts). This is the end of our derivation. We have shown that the microscopic description of open quantum system, based on the weak coupling limit approach, can be considered compatible with our previous, purely mathematical one, where the *complete positivity* was not derived from the base principles, but rather assumed as a paradigm.

9. Examples of Markovian Master Equations

In this section we will provide some brief examples of Markovian Master Equations and their solutions. In order to remain as simple and clear as possible we will be mainly focused on low-dimensional systems, such as two-level system. We will also restrict ourselves to exactly solvable models only.

9.1. Two-level system and its decay

Our first and the most illuminating example is the simplest one: the two-level system, which is allowed to interact with electromagnetic field, which remains in an equilibrium state of temperature T. We recall that such electromagnetic field can be described with the use of so-called *Bose-Einstein distribution function*,

$$N(\omega) = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1},$$

where $N(\omega)$ is the average number of photons in a mode of frequency ω and k_B is the Boltzmann constant. Our system will be assumed to be so simple, that it has only two possible states: the **ground state** and the **excited state**. This means, that the Hilbert space of the system is simply $\mathbb{C}^2$, in which we select an orthonormal basis $\{\varphi_0, \varphi_1\}$ given simply as

$$\varphi_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad \varphi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

where φ_0 corresponds to the ground state and φ_1 to the excited state. These two vectors are the eigenvectors of system's Hamiltonian,

$$H\varphi_0 = E_0\varphi_0, \qquad H\varphi_1 = E_1\varphi_1,$$

where E_0 and E_1 are the energies of ground and excited state, respectively. It is convenient to work in customarily chosen energy scale, such that the energy of ground state and energy of excited state are equally distanced from 0. We achieve this via the transformation

$$H \;\mapsto\; H' = H - \frac{1}{2}(E_1 + E_0)I.$$

The Reader can now check that such transformed Hamiltonian H' commutes with H and has the same eigenvectors, however now corresponding to new eigenenergies,

$$E_0' = -\frac{E_1 - E_0}{2} = -\frac{\hbar\omega_0}{2}, \qquad E_1' = \frac{E_1 - E_0}{2} = \frac{\hbar\omega_0}{2}$$

where we introduced $\omega_0 = \frac{E_1 - E_0}{\hbar}$, the transition frequency between states. This means that H' is diagonal in this basis,

$$H' = E_0'|\varphi_0\rangle\langle\varphi_0| + E_1'|\varphi_1\rangle\langle\varphi_1| = \frac{\hbar\omega_0}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar\omega_0}{2}\sigma_3,$$

where we employed Dirac's *bra-ket notation* and $\sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ is one of the Pauli matrices (compare with Section 2.1.1). We also define two matrices,

$$\sigma_+ = \frac{1}{2}(\sigma_1 + i\sigma_2) = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}, \qquad \sigma_- = \frac{1}{2}(\sigma_1 - i\sigma_2) = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix},$$

called the *raising* and *lowering operator*, respectively (why are they called so?). The density matrix of such two-level system will be then given in basis $\{\varphi_0, \varphi_1\}$ as

$$\rho_t = \begin{pmatrix}\rho_{11}(t) & \rho_{10}(t)\\ \rho_{01}(t) & \rho_{00}(t)\end{pmatrix}.$$

Terms $\rho_{00}(t)$ and $\rho_{11}(t) = 1 - \rho_{00}(t)$, called the **populations**, describe probabilities of our system to be respectively in the ground or the excited state. Off-diagonal terms $\rho_{10}(t)$ and $\rho_{01}(t) = \overline{\rho_{10}(t)}$, called the **coherences**, encode information on the transitions between ground and excited state and are commonly understood as a measure of *non-classicality* of the entire mixed state[15].

The Markovian Master Equation of such a system can be then expressed (we omit the derivation) in the interaction picture in a form

$$\frac{d\rho_t}{dt} = L(\rho_t) = \gamma_0\left(\sigma_-\rho_t\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_t\}\right) + \gamma_0 N(\omega_0)\left(\sigma_-\rho_t\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_t\}\right)$$
$$+\gamma_0 N(\omega_0)\left(\sigma_+\rho_t\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho_t\}\right),$$

where γ_0 is the rate of spontaneous emission which may be found to be

$$\gamma_0 = \frac{4\omega_0^3\left|\vec{d}\right|^2}{3\hbar c^3},$$

for $\vec{d}$ being the vector of *electric dipole moment* (its appearance originates from the chosen form of the interaction Hamiltonian between system and the electromagnetic field – see [5] for extensive details). The Master Equation consists therefore of three terms: the first one describes process of **spontaneous emission** of the two-level system and therefore its transition from excited state to the ground state; the second and third one in turn describe thermally induced processes of **emission** and **absorption**, respectively.

9.1.1. Evolution and return to equilibrium

The Master Equation of such two-level system may seem complicated but in reality, it is quite easy to deal with its right hand side since operators $\sigma_\pm$ are extremally simple. The Reader can check, by quite simple computation, that the resulting equation is

$$\frac{d\rho_t}{dt} = L(\rho_t) = \begin{pmatrix}\dot{\rho}_{11}(t) & \dot{\rho}_{10}(t)\\ \dot{\rho}_{01}(t) & \dot{\rho}_{00}(t)\end{pmatrix}$$

[15] If, for instance both coherences are 0, then the mixed state is interpreted as purely classical probability distribution of pure states. If, on the other hand they are nonzero, this means that the mixed state has nonclassical properties.

$$= \begin{pmatrix} \gamma_0 N(\omega_0) - \gamma_0\big(1+2N(\omega_0)\big)\rho_{11}(t) & -\frac{\gamma_0}{2}\big(1+2N(\omega_0)\big)\rho_{10}(t) \\ -\frac{\gamma_0}{2}\big(1+2N(\omega_0)\big)\rho_{01}(t) & -\dot{\rho}_{11}(t) \end{pmatrix}$$

which comes by the trace preservation condition, $\rho_{00}(t)+\rho_{11}(t)=1$. It is also not hard to find the actual solution of this equation – you can check that it is of a form

$$\rho_{11}(t) = \frac{N(\omega_0)}{1+2N(\omega_0)} + \left(\rho_{11}(0) - \frac{N(\omega_0)}{1+2N(\omega_0)}\right) e^{-\gamma_0(1+2N(\omega_0))t},$$

$$\rho_{01}(t) = \rho_{01}(0) e^{-\frac{1}{2}\gamma_0(1+2N(\omega_0))t},$$

$$\rho_{10}(t) = \overline{\rho_{01}(0)} e^{-\frac{1}{2}\gamma_0(1+2N(\omega_0))t},$$

$$\rho_{00}(t) = 1 - \rho_{11}(t).$$

Now, since both $\gamma_0, N(\omega_0) > 0$ we see that the state ρ_t tends asymptotically (i.e. when $t \to \infty$) to a matrix

$$\rho_\infty = \begin{pmatrix} \frac{N(\omega_0)}{1+2N(\omega_0)} & 0 \\ 0 & \frac{1+N(\omega_0)}{1+2N(\omega_0)} \end{pmatrix}$$

which can be checked to be the *thermal equilibrium state*, i.e. a state of a form

$$\rho_\beta = \frac{e^{-\beta H}}{\operatorname{tr} e^{-\beta H}}, \qquad \beta = \frac{1}{k_B T}.$$

Such state is also a stationary state of the dynamics, namely it satisfies $L(\rho_\beta) = 0$ (verify it!).

9.2. Two-level system with resonant driving

In this example, we modify the previous case by adding another, external source of coherent and monochromatic light of frequency adjusted to the two level system's own frequency ω_0. Namely, we assume that the system is additionally driven by a laser source in resonance with the transition between ground and excited state. It can be justified that the Hamiltonian of interaction between two level system and such monochromatic wave can be put in so-called *dipole approximation* as

$$H_L = -\vec{D}(t)\cdot\vec{E}(t),$$

where $\vec{D}(t) = \vec{d}\sigma_- e^{-i\omega_0 t} + \vec{d}^*\sigma_+ e^{i\omega_0 t}$ is the interaction picture version of the electric dipole moment operator and

$$\vec{E}(t) = \vec{\mathcal{E}} e^{-i\omega_0 t} + \vec{\mathcal{E}}^* e^{i\omega_0 t}$$

is the electric field vector of a driving laser light. Performing the calculation,

$$\begin{aligned} H_L = -\vec{D}(t)\cdot\vec{E}(t) &= -\big(\vec{d}\sigma_- e^{-i\omega_0 t} + \vec{d}^*\sigma_+ e^{i\omega_0 t}\big)\cdot\big(\vec{\mathcal{E}} e^{-i\omega_0 t} + \vec{\mathcal{E}}^* e^{i\omega_0 t}\big) \\ &= -\big(\vec{d}\cdot\vec{\mathcal{E}}\big)e^{-2i\omega_0 t}\sigma_- - \big(\vec{d}\cdot\vec{\mathcal{E}}^*\big)\sigma_- - \big(\vec{d}^*\cdot\vec{\mathcal{E}}\big)\sigma_+ - \big(\vec{d}^*\cdot\vec{\mathcal{E}}^*\big)e^{2i\omega_0 t}. \end{aligned}$$

Now we apply something what is known in literature as the Rotating Wave Approximation: namely, we notice that time-dependent terms in the above expression oscillate really rapidly and so, after averaging, their contribution to the behaviour of the system can be neglected. Therefore we simply omit them and get

$$H_L = -\big(\vec{d}\cdot\vec{\mathcal{E}}^*\big)\sigma_- - \big(\vec{d}^*\cdot\vec{\mathcal{E}}\big)\sigma_+.$$

It is common to introduce the so-called Rabi frequency

$$\Omega = 2\vec{d}^* \cdot \vec{\mathcal{E}},$$

so the Hamiltonian becomes

$$H_L = -\frac{1}{2}\bar{\Omega}\sigma_- - \frac{1}{2}\Omega\sigma_+.$$

In order to simplify the situation, we can assume that the phase of external field was chosen in such a way, that Ω becomes real and positive, so

$$H_L = -\frac{1}{2}\Omega(\sigma_- + \sigma_+).$$

Ang again, one can check that the resulting Markovian Master Equation of such resonantly driven two-level system immersed in an electromagnetic reservoir in thermal state (in the interaction picture) becomes

$$\frac{d\rho_t}{dt} = L(\rho_t) = \frac{i\Omega}{2}[\sigma_- + \sigma_+, \rho_t] + \gamma_0\left(\sigma_-\rho_t\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_t\}\right) + \gamma_0 N(\omega_0)\left(\sigma_-\rho_t\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_t\}\right) + \gamma_0 N(\omega_0)\left(\sigma_+\rho_t\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho_t\}\right),$$

i.e. almost the same, as before.

9.2.1. Electrooptical Bloch equations

There is yet another, really convenient way of describing evolution of two-level systems. Notice that in general, the density matrix of such system is a 2-by-2 matrix and so is an element from $M_2(\mathbb{C})$ vector space. We have already said, back in Section 2.1.1, that the Pauli matrices σ_i constitute for a basis in $M_2(\mathbb{C})$ which is orthogonal, but not orthonormal. This means that one can expand ρ_t in such basis,

$$\rho_t = \sum_{i=1}^{4} \alpha_i(t)\sigma_i,$$

for some (complex) coefficients $\alpha_i(t)$. We remember that trace of ρ_t must be 1, so we have

$$1 = \operatorname{tr}\rho_t = \operatorname{tr}\sum_{i=1}^{4} \alpha_i(t)\sigma_i = \sum_{i=1}^{4} \alpha_i(t)\operatorname{tr}\sigma_i = \alpha_4(t)\operatorname{tr}\sigma_4 = 2\alpha_4(t),$$

since all Pauli matrices, apart from σ_4, are traceless; this means, that the coefficient $\alpha_4(t)$ must be constant,

$$\alpha_4(t) = \frac{1}{2}.$$

On the other hand, density matrix ρ_t must also be a Hermitian matrix, so $\rho_t = \rho_t^*$. This yields

$$\rho_t^* = \left(\sum_{i=1}^{4} \alpha_i(t)\sigma_i\right)^* = \sum_{i=1}^{4} \overline{\alpha_i(t)}\sigma_i^* = \sum_{i=1}^{4} \overline{\alpha_i(t)}\sigma_i = \rho_t$$

since all Pauli matrices are Hermitian; this however means that $\alpha_i(t) = \overline{\alpha_i(t)}$ so all coefficients $\alpha_i(t)$ must be real. Now recall, from Theorem 18, that we have $\operatorname{tr}\rho_t^2 \leq 1$; this means that

$$1 \geq \operatorname{tr}\left(\sum_{i=1}^{4} \alpha_i(t)\sigma_i\right)^2 = \operatorname{tr}\sum_{i,j=1}^{4} \alpha_i(t)\alpha_j(t)\sigma_i\sigma_j = \sum_{i,j=1}^{4} \alpha_i(t)\alpha_j(t)\operatorname{tr}\sigma_i\sigma_j = 2\sum_{i=1}^{4} \alpha_i(t)^2$$

which comes by the fact, that $\operatorname{tr}\sigma_i\sigma_j = 2\delta_{ij}$ (verify it!). This, together with $r_4(t) = \frac{1}{2}$ yields

$$1 \geq 2\left(\frac{1}{4}+\sum_{i=1}^{3}\alpha_i(t)^2\right) \;\Rightarrow\; \frac{1}{4}\geq\sum_{i=1}^{3}\alpha_i(t)^2=|\vec{\alpha}(t)|^2,$$

where we introduced a real, 3-dimensional time-dependent vector $\vec{\alpha}(t)=\big(\alpha_1(t),\alpha_2(t),\alpha_3(t)\big)$. Now we can rewrite everything in order to obtain

$$\rho_t=\sum_{i=1}^{4}\alpha_i(t)\sigma_i=\frac{1}{2}I+\sum_{i=1}^{3}\alpha_i(t)\sigma_i=\frac{1}{2}\left(I+\sum_{i=1}^{3}r_i(t)\sigma_i\right),$$

for a new vector (verify it!)

$$\vec{r}(t)=2\vec{\alpha}(t), \qquad r_i(t)=\operatorname{tr}\sigma_i\rho_t.$$

By the earlier computation we see however, that this vector's norm must be bounded,

$$|\vec{r}(t)|^2=4|\vec{\alpha}(t)|^2\leq 4\cdot\frac{1}{4}=1.$$

Such a vector $\vec{r}(t)$ is commonly called **the Bloch vector** and it describes the density matrix in a unique way. The reality shows that the Bloch vector formalism allows for possibly the easiest description of two-level systems and therefore it appears very broadly in literature. In fact, every Master Equation for ρ_t can be re-expressed as a differential equation for corresponding Bloch vector; we encourage Reader to check, that our Master Equation translates into a linear nonhomogeneous ordinary differential equation

$$\frac{d\vec{r}(t)}{dt}=G\vec{r}(t)+\vec{b},$$

where $G\in M_3(\mathbb{C})$ and $\vec{b}\in\mathbb{R}^3$ are

$$G=\begin{pmatrix}-\gamma/2 & 0 & 0\\ 0 & -\gamma/2 & \Omega\\ 0 & -\Omega & -\gamma\end{pmatrix}, \qquad \vec{b}=\begin{pmatrix}0\\0\\-\gamma_0\end{pmatrix},$$

where we put $\gamma=\gamma_0(2N(\omega_0)+1)$ for short. The last vector differential equation is sometimes called in literature the (system of) **electrooptical Bloch equation**.

9.3. Damped harmonic oscillator

This is our final example, however it is a tricky one. Earlier on, we have made a simplifying assumption of our open systems in question to be finite dimensional. Here, we explicitly break this assumption: namely, we consider a system S being the **harmonic oscillator** of some internal frequency ω_0, or, equivalently, a box, which can absorb any number of photons of frequency ω_0. Each absorbed photon raises the energy of a system by $\hbar\omega_0$ and each emitted one lowers the energy by $\hbar\omega_0$. We introduce here a standard formalism of creation and annihilation operators. Namely, let

$$\varphi_n=(0,\ldots,0,\underbrace{1}_{n},0,\ldots), \quad n\in\mathbb{N}$$

be a vector with 1 in the n-th slot and 0's everywhere else. One can show that a set $\{\varphi_n : n\in\mathbb{N}\}$ of all such vectors constitute for an orthonormal basis in Hilbert space l^2 of square-summable sequences. Our interpretation of such vectors is that vector φ_n matches the situation of the box containing exactly n absorbed photons[16]. On this Hilbert space, we introduce two linear operators a and a^* acting via a prescription

[16] Such basis is sometimes called the *occupancy number representation*.

$$a^*\varphi_n = \sqrt{n+1}\varphi_{n+1}, \qquad a\varphi_n = \sqrt{n}\varphi_{n-1}, \qquad a\varphi_0 = 0.$$

Operator a, called the *annihilation operator*, effectively (up to a constant) removes photon (and energy) from the box, while a^*, called the *creation operator*, adds a photon. It is easy to check, that φ_n are the eigenvectors of an operator a^*a,

$$a^*a\varphi_n = n\varphi_n,$$

for eigenvalue n; such operator then encodes a total number of photons inside a box, or equivalently a number of eigenstate of the oscillator and is therefore called the *particle number operator*. The total energy of the oscillator then equals the total energy of all absorbed photons, which must be then n times the energy of one photon, which is $\hbar\omega_0$; this means, that the oscillator's Hamiltonian operator is

$$H = \hbar\omega_0 a^*a.$$

For the environment, we can again take electromagnetic field in thermal equilibrium, described by Bose-Einstein distribution function $N(\omega) = \left(e^{\hbar\omega/k_BT} - 1\right)^{-1}$. The Master Equation of such harmonic oscillator can be then found to be, in Schrödinger picture,

$$\frac{d\rho_t}{dt} = L(\rho_t) = -i\omega_0[a^*a, \rho_t] + \gamma_0(N(\omega_0)+1)\left(a\rho_t a^* - \frac{1}{2}\{a^*a, \rho_t\}\right) + \gamma_0 N(\omega_0)\left(a^*\rho_t a - \frac{1}{2}\{aa^*, \rho_t\}\right),$$

where the commutator term describes system's own evolution (without influence from the reservoir), the second and third term describe processes of respectively spontaneous and induced emission of a photon from the box into the reservoir and the last term describes a process of absorption of a photon from the environment into the box.

9.3.1. Adjoint Master Equation

We will not provide an explicit solution of the above equation. Instead, we will try to find the time dependence of a mean number of photons inside the box. For this, we introduce a notion of *adjoint Master Equation*. Recall, that the time-dependent expectation (average) value of some operator A acting on Hilbert space of the system was given by equation

$$\langle A(t)\rangle = \operatorname{tr}\rho_t A.$$

Remember, that the evolution of ρ_t was determined by quantum dynamical map Λ_t, which was from the very beginning assumed completely positive and trace preserving; this means that one can always put Λ_t into its Kraus form as

$$\Lambda_t(\rho_0) = \sum_\alpha V_\alpha(t)\rho_0 V_\alpha(t)^*$$

for some family of time-dependent bounded operators $\{V_\alpha(t)\}$. If we put this into the expectation value and apply cyclic property of trace we obtain

$$\langle A(t)\rangle = \operatorname{tr}\Lambda_t(\rho_0)A = \operatorname{tr}\sum_\alpha V_\alpha(t)\rho_0 V_\alpha(t)^* A = \operatorname{tr}\rho_0 \sum_\alpha V_\alpha(t)^* A V_\alpha(t) = \operatorname{tr}\rho_0 A_H(t),$$

where we introduced a new time-dependent linear operator

$$A_H(t) = \sum_\alpha V_\alpha(t)^* A V_\alpha(t) = \Lambda_t^*(A)$$

Such operator $A_H(t)$ is called the **Heisenberg picture** of operator A and linear map Λ_t^* is called the **dual map** of Λ_t. In many situations it is indeed easier to work in the Heisenberg picture first, and then "transform" the results back to the original Schrödinger picture; this is what we will do now.

The Heisenberg picture of A satisfies differential equation

$$\frac{d}{dt}A_H(t) = \sum_\alpha \left(\frac{dV_\alpha(t)^*}{dt} A V_\alpha(t) + V_\alpha(t)^* A \frac{dV_\alpha(t)}{dt} \right).$$

On the other hand, using again properties of trace,

$$\begin{aligned}
\operatorname{tr} \rho_0 \frac{dA_H(t)}{dt} &= \operatorname{tr}\left[\rho_0 \sum_\alpha \left(\frac{dV_\alpha(t)^*}{dt} A V_\alpha(t) + V_\alpha(t)^* A \frac{dV_\alpha(t)}{dt} \right) \right] \\
&= \operatorname{tr}\left[\sum_\alpha \left(V_\alpha(t) \rho_0 \frac{dV_\alpha(t)^*}{dt} + \frac{dV_\alpha(t)}{dt} \rho_0 V_\alpha(t)^* \right) A \right] \\
&= \operatorname{tr}\left[\frac{d}{dt} \sum_\alpha V_\alpha(t) \rho_0 V_\alpha(t)^* A \right] = \operatorname{tr}\left[\frac{d\rho_t}{dt} A \right] = \operatorname{tr} L_t(\rho_t) A,
\end{aligned}$$

so dynamics of $A_H(t)$ is also indirectly governed by L_t. This means that in order to find $\frac{dA_H(t)}{dt}$, we have to adjust operators appearing in $L_t(\rho_t)$ utilizing properties of trace:

$$\begin{aligned}
\operatorname{tr} \rho_0 \frac{dA_H(t)}{dt} &= \operatorname{tr} L_t(\rho_t) A \\
&= \operatorname{tr}\left[\left(-i[H_t, \rho_t] + \sum_\alpha \left(X_\alpha(t) \rho_t X_\alpha(t)^* - \frac{1}{2}\{X_\alpha(t)^* X_\alpha(t), \rho_t\} \right) \right) A \right] \\
&= \operatorname{tr}\Bigg[-i(H_t \rho_t A - \rho_t H_t A) \\
&\quad + \sum_\alpha \left(X_\alpha(t) \rho_t X_\alpha(t)^* A - \frac{1}{2} X_\alpha(t)^* X_\alpha(t) \rho_t A - \frac{1}{2} \rho_t X_\alpha(t)^* X_\alpha(t) A \right) \Bigg] \\
&= \operatorname{tr}\Bigg[-i\rho_t(A H_t - H_t A) \\
&\quad + \rho_t \sum_\alpha \left(X_\alpha(t)^* A X_\alpha(t) - \frac{1}{2} A X_\alpha(t)^* X_\alpha(t) - \frac{1}{2} X_\alpha(t)^* X_\alpha(t) A \right) \Bigg] \\
&= \operatorname{tr}\left[\rho_t \left(-i[A, H_t] + \sum_\alpha \left(X_\alpha(t)^* A X_\alpha(t) - \frac{1}{2}\{X_\alpha(t)^* X_\alpha(t), A\} \right) \right) \right] \\
&= \operatorname{tr}\left[\rho_t \left(i[H_t, A] + \sum_\alpha \left(X_\alpha(t)^* A X_\alpha(t) - \frac{1}{2}\{X_\alpha(t)^* X_\alpha(t), A\} \right) \right) \right] \\
&= \operatorname{tr}[\rho_t L_t^*(A)],
\end{aligned}$$

where we introduced a map L_t^*, dual to L_t,

$$L_t^*(A) = i[H_t, A] + \sum_\alpha \left(X_\alpha(t)^* A X_\alpha(t) - \frac{1}{2}\{X_\alpha(t)^* X_\alpha(t), A\} \right).$$

This allows to write, after putting $\rho_t = \sum_\alpha V_\alpha(t) \rho_0 V_\alpha(t)^*$ and reordering,

$$\operatorname{tr} \rho_0 \frac{dA_H(t)}{dt} = \operatorname{tr}[\rho_t L_t^*(A)] = \operatorname{tr}[\rho_0 \Lambda_t^* L_t^*(A)],$$

from which we deduce expression for $\frac{dA_H(t)}{dt}$ to be given by

$$\frac{dA_H(t)}{dt} = \Lambda_t^* L_t^*(A).$$

Now, if it is true that L_t is constant, then naturally $\Lambda_t = e^{tL}$ and L, Λ_t commute. The same is then true for their duals, so if $L_t = \text{const}$ then also $L_t^* = L^*$ is constant and commutes with $\Lambda_t^* = e^{tL^*}$; if this is the case, we have

$$\begin{aligned}\frac{dA_H(t)}{dt} &= \Lambda_t^* L^*(A) = L^* \Lambda_t^*(A) = L^*\big(A_H(t)\big) \\ &= i[H, A_H(t)] + \sum_\alpha \left(X_\alpha^* A_H(t) X_\alpha - \frac{1}{2}\{X_\alpha^* X_\alpha, A_H(t)\}\right),\end{aligned}$$

which is the equation of motion of operators in the Heisenberg picture, called the **adjoint Master Equation**.

9.3.2. Return to equilibrium

But, since $A_H(t) = \Lambda_t^*(A) = e^{tL^*}(A)$, we have to compute the exponential of tL^* first and specify how it acts on A. This is achieved by using a power series expansion,

$$e^{tL^*} = \sum_{n=0}^{\infty} \frac{t^n (L^*)^n}{n!}.$$

To exemplify, we will compute explicitly the Heisenberg picture of annihilation and creation operators a, a^* in our example of harmonic oscillator. The dual map L^* reads

$$\begin{aligned}L^*(A) = i\omega_0[a^*a, A] + \gamma_0(N(\omega_0)+1)\left(a^*Aa - \frac{1}{2}\{a^*a, A\}\right) \\ +\gamma_0 N(\omega_0)\left(aAa^* - \frac{1}{2}\{aa^*, A\}\right).\end{aligned}$$

Let us calculate $L^*(a)$:

$$\begin{aligned}L^*(a) = i\omega_0[a^*a, a] + \gamma_0(N(\omega_0)+1)\left(a^*aa - \frac{1}{2}\{a^*a, a\}\right) \\ +\gamma_0 N(\omega_0)\left(aaa^* - \frac{1}{2}\{aa^*, a\}\right).\end{aligned}$$

First, we will reorder this expression,

$$\begin{aligned}L^*(a) &= i\omega_0[a^*a, a] + \gamma_0(N(\omega_0)+1)\left(a^*aa - \frac{1}{2}a^*aa - \frac{1}{2}aa^*a\right) \\ &+\gamma_0 N(\omega_0)\left(aaa^* - \frac{1}{2}aa^*a - \frac{1}{2}aaa^*\right) \\ &= i\omega_0[a^*a, a] + \gamma_0(N(\omega_0)+1)\left(\frac{1}{2}a^*aa - \frac{1}{2}aa^*a\right) \\ &+\gamma_0 N(\omega_0)\left(\frac{1}{2}aaa^* - \frac{1}{2}aa^*a\right) \\ &= i\omega_0[a^*a, a] + \frac{1}{2}\gamma_0(N(\omega_0)+1)[a^*a, a] + \frac{1}{2}\gamma_0 N(\omega_0)[a, aa^*].\end{aligned}$$

The reason, why we did this is that now we can apply well-known commutation relation (check it!)

$$[a, a^*] = I$$

as well as the following properties of commutators (check it also…!)

$$[A, B] = -[B, A], \qquad [AB, C] = [A, C]B + A[B, C],$$

in order to achieve, after some easy algebra (…and this!),

$$[a^*a, a] = -a, \qquad [a, aa^*] = a,$$

yielding (yes, this one too!)

$$L^*(a) = -\left(i\omega_0 + \frac{\gamma_0}{2}\right) a = -\xi a.$$

This result shows that the only action of L^* on a is the rescaling of the original operator. By induction (do this!) we therefore see, that

$$(L^*)^n(a) = (-\xi)^n a,$$

and so we obtain

$$a_H(t) = e^{tL^*}(a) = \sum_{n=0}^{\infty} \frac{t^n}{n!}(L^*)^n(a) = \sum_{n=0}^{\infty} \frac{t^n(-\xi)^n}{n!} a = e^{-\xi t} a = e^{-\left(i\omega_0 + \frac{\gamma_0}{2}\right)t} a.$$

By the very same methods, one also quickly finds Heisenberg pictures of a^* and the particle number operator,

$$a_H^*(t) = e^{\left(i\omega_0 - \frac{\gamma_0}{2}\right)t} a^*, \qquad (a^*a)_H(t) = e^{-\gamma_0 t} a^*a + N(\omega_0)(1 - e^{-\gamma_0 t}).$$

Now, what this computation tells us is that that the mean amplitude of the oscillator $\langle a(t)\rangle$ and the mean number of photons inside the box $\langle (a^*a)(t)\rangle$ are, according to the very start of this section,

$$\langle a(t)\rangle = \operatorname{tr} \rho_0 a_H(t) = e^{-\left(i\omega_0 + \frac{\gamma_0}{2}\right)t} \langle a\rangle,$$
$$\langle (a^*a)(t)\rangle = \operatorname{tr} \rho_0 (a^*a)_H(t) = e^{-\gamma_0 t} \langle a^*a\rangle + N(\omega_0)(1 - e^{-\gamma_0 t}).$$

The mean oscillator's amplitude then vanishes exponentially in time (following an exponential spiral curve on the complex plane). Ater a time long enough, so in the limit $t \to \infty$, we therefore have

$$\lim_{t\to\infty} \langle a(t)\rangle = 0, \qquad \lim_{t\to\infty} \langle (a^*a)(t)\rangle = N(\omega_0).$$

This means, that after vey long time, the harmonic oscillator dissipates its energy and tends to a stable equilibrium state such that the mean number of photons inside the box does not change and is specified not by properties of the oscillator, but rather by properties of the reservoir.