TCM315 Fall 2022: Introduction to Open Quantum Systems

Lecture 5: State operator and geometry

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INTRODUCTION

These introductory notes on state operators and their elementary properties draw from chapter 3 of [4]. A more advanced textbook on the geometry of quantum states is [2].

STATE OPERATOR

The first postulate states that complete information about a physical system is embodied by a unit ray $\boldsymbol{\psi}$ in the Hilbert space $\mathcal{H}$. Given a system represented by state vector $\boldsymbol{\psi}$, the probability to measure the i-th eigenvalue of the self-adjoint operator $\mathbb{A}$ with **non-degenerate spectrum** and associated to the dynamical variable $\mathscr{A}$ is

$$\mathrm{P}\left(\mathscr{A}=\alpha_i \middle| \boldsymbol{\psi}\right)=\left\|\boldsymbol{a}_i^{\dagger}\boldsymbol{\psi}\right\|^2 \tag{1}$$

if

$$\mathbb{A}\boldsymbol{a}_i=\alpha_i\boldsymbol{a}_i$$

The spectral theorem also tells us that we can represent $\mathbb{A}$ as the linear combination of the projectors along the linear subspaces spanned by the eigenvectors $\{\boldsymbol{a}_i\}_{i=1}^{d}$:

$$\mathbb{A}=\sum_{i=1}^{d}\alpha_i\mathbb{P}_i \tag{2}$$

In the **non-degenerate** case the projectors are uniquely specified by the outer (column by row) product of the eigenvectors

$$\mathbb{P}_i = \boldsymbol{a}_i \boldsymbol{a}_i^{\dagger}$$

Similarly, we avail us of the outer product to uniquely associate to any unit ray a projector operator

$$\boldsymbol{\rho} = \boldsymbol{\psi}\boldsymbol{\psi}^{\dagger}$$

Once we adopt these conventions, we readily verify that the probability (1) admits representation

$$\mathrm{P}\left(\mathscr{A} = \alpha_i \middle| \boldsymbol{\rho} = \boldsymbol{\psi}\boldsymbol{\psi}^{\dagger}\right) = \mathrm{Tr}\left(\boldsymbol{\rho}\, \mathbb{P}_i\right) \tag{3}$$

This latter representation has some immediate advantages.

Degenerate case

First, we immediately recover the content of the second postulate in the case of degenerate eigenvalues when the sum over projectors in (2) is restricted to $\mathscr{N} < d$ distinct eigenvalues.

$$\mathbb{A} = \sum_{i=1}^{\mathscr{N}} \alpha_i \mathbb{P}_i$$

Epistemic probabilities

We can encompass in the formalism **mixtures** of states

$$\boldsymbol{\rho} = \sum_{i=1}^{\mathscr{M}} \wp_i\, \boldsymbol{\psi}_i \boldsymbol{\psi}_i^{\dagger} \tag{4}$$

weighed by collections $\{\wp_i\}_{i=1}^{\mathscr{M}}$ of **epistemic probabilities** quantifying the experimenter's degree of knowledge (or ignorance) on the exact state of the system e.g. upon repeating the same experiment. Clearly the $\wp_i$'s must satisfy

$$\wp_i \geq 0 \qquad \text{for all}\, i = 1, \dots, \mathscr{M} \tag{5a}$$

$$\sum_{i=1}^{\mathscr{M}} \wp_i = 1 \tag{5b}$$

The a **state operator** defined by (4) satisfies

P-1 $\boldsymbol{\rho} = \boldsymbol{\rho}^{\dagger}$ (in the infinite dimensional case self-adjointness requires $\mathrm{dom}(\boldsymbol{\rho}) = \mathrm{dom}(\boldsymbol{\rho}^{\dagger})$). Namely,

$$\boldsymbol{\rho}^{\dagger} = \left(\sum_{i=1}^{\mathscr{M}} \wp_i\, \boldsymbol{\psi}_i \boldsymbol{\psi}_i^{\dagger}\right)^{\dagger} = \sum_{i=1}^{\mathscr{M}} \wp_i\, \boldsymbol{\psi}_i \boldsymbol{\psi}_i^{\dagger}$$

as the $\wp_i$'s are real.

P-2 $\mathrm{Sp}(\boldsymbol{\rho}) \geq 0$. Namely, for any $\boldsymbol{v} \in \mathcal{H}$

$$\boldsymbol{v}^{\dagger}\boldsymbol{\rho}\boldsymbol{v} = \sum_{i=1}^{\mathscr{M}} \wp_i\, \|\boldsymbol{\psi}_i^{\dagger}\boldsymbol{v}\|^2 \geq 0$$

by (5a). We conclude that $\boldsymbol{\rho}$ is positive definite and therefore has positive define **spectrum**.

P-3 $\mathrm{Tr}(\boldsymbol{\rho}) = 1$. Namely,

$$\mathrm{Tr}(\boldsymbol{\rho}) = \sum_{i=1}^{\mathscr{N}} \wp_i \ \mathrm{Tr}\left(\boldsymbol{\psi}_i \boldsymbol{\psi}_i^\dagger\right) = \sum_{i=1}^{\mathscr{N}} \wp_i \ \|\boldsymbol{\psi}_i\|^2 = \sum_{i=1}^{\mathscr{N}} \wp_i = 1$$

by (5b).

The properties (**P-1**), (**P-2**) and (**P-3**) are necessary and sufficient to specify a mixture. Namely, the spectral theorem guarantees that an operator enjoying the self-adjoint property (**P-1**) is always amenable to the form

$$\boldsymbol{\rho} = \sum_{i=1}^{\mathscr{N}} r_i \mathbb{P}_{r_i}$$

the $\mathbb{P}_{r_i}$'s being the projectors on the orthogonal sub-spaces associated to the distinct eigenvalues r_i of dimensions

$$\mathrm{Tr}\,\mathbb{P}_{r_i} = d_i \qquad \text{with} \qquad \sum_{i=1}^{\mathscr{N}} d_i = d$$

The remaining properties (**P-2**), (**P-3**) ensure the interpretation of the quantities

$$\wp_i = r_i\, d_i$$

as probabilities.

Liouville-von Neumann equation

The unitary evolution postulate determines the evolution of the state operator. Namely,

$$\boldsymbol{\psi}_{t_2} = \mathbb{U}_{t_2,t_1}\, \boldsymbol{\psi}_{t_1}$$

implies

$$\boldsymbol{\rho}_{t_2} = \mathbb{U}_{t_2,t_1} \boldsymbol{\rho}_{t_1} \mathbb{U}_{t_2,t_1}^\dagger \tag{6}$$

and vice versa. The differential form of (6) is the Liouville-von Neumann equation

$$\imath\, \partial_t \boldsymbol{\rho}_t = [\mathbb{H}_t\,, \boldsymbol{\rho}_t]$$

$$\boldsymbol{\rho}_0 = \sum_{i=1}^{\mathscr{M}} c_i \boldsymbol{\psi}_{0,i} \boldsymbol{\psi}_{0,i}^\dagger$$

with $\mathscr{M} \geq 1$ an arbitrary, context depending integer, and the coefficients $\{c_i\}_{i=1}^{\mathscr{M}}$ satisfying the conditions (5).

Measurement

In terms of the state operator the generalised measurement postulate must be rephrased considering again a collection of measurement operators $\{\mathbb{M}_i\}_{i\geq 1}^{\mathscr{M}}$ and satisfying the **completeness equation**:

$$\sum_{i=1}^{\mathscr{M}} \mathbb{M}_i^\dagger \mathbb{M}_i = \mathbb{1}_d$$

The measurement of the outcome of the experiment associated to the operator $\mathbb{M}_i$ then occasions the instantaneous collapse of the state operator to the **post- measurement** values $\{\boldsymbol{\rho}_i\}_{i=1}^{\mathscr{M}}$ defined in accordance to the measurement postulate

$$\boldsymbol{\rho} \mapsto \boldsymbol{\rho}_i = \frac{\mathbb{M}_i\, \boldsymbol{\rho}\, \mathbb{M}_i^\dagger}{\mathrm{Tr}\left(\mathbb{M}_i\, \boldsymbol{\rho}\, \mathbb{M}_i^\dagger\right)}$$

The probability of measuring the outcome is

$$\wp_i = \mathrm{Tr}\left(\mathbb{M}_i\, \boldsymbol{\rho}\, \mathbb{M}_i^\dagger\right)$$

QUANTUM STATE OPERATORS AS A CONVEX SET

We have seen that a state operator acting on an Hilbert space is characterized by the properties (**P-1**)-(**P-2**), (**P-3**). Given a state operator $\boldsymbol{\rho}$, we are now interested in determining whether $\boldsymbol{\rho}$ specifies a **pure state** or is instead a **mixed state** as (4) for any $\mathscr{M} > 1$.

Definition. *We call **pure** any state operator amenable to the form of a projector along a unit vector $\boldsymbol{\psi}$ of the Hilbert space*

$$\boldsymbol{\rho} = \boldsymbol{\psi}\boldsymbol{\psi}^{\dagger} \equiv \mathbb{P}_{\psi}$$

It is a straightforward exercise to prove that a **state operator** is pure **if and only if**

$$\operatorname{Tr} \boldsymbol{\rho}^2 = 1$$

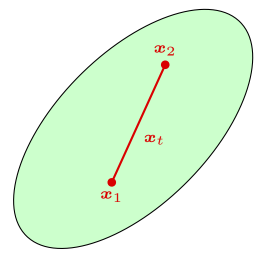
It is useful to **geometrically** characterize pure states as the extremal elements, i.e. the elements lying on the boundary, of the **convex set** comprising all the possible state operators in an Hilbert space. To start with we recall that the space $\mathcal{M}_d(\mathbb{C})$ of the matrices acting on a d dimensional vector space is itself a d^2-dimensional complex vector space.

Definition. *A subset* S *of a vector space is a **convex set** if for any pair of points $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ belonging to the set it is true that the mixture $\boldsymbol{x}_t$ also belongs to the set, i.e. the **linear combination***

$$\boldsymbol{x}_t = t\,\boldsymbol{x}_1 + (1-t)\,\boldsymbol{x}_0$$

belongs to S *for all t in the unit interval*

$$t \in [0,1]$$



Stylized convex set

Pure states are extremal of a convex set

Proposition. *The Hilbert–Schmidt inner product of two states $\boldsymbol{\rho}_{(i)}$ $i = 1, 2$ must satisfy*

$$0 \leq \operatorname{Tr}(\boldsymbol{\rho}_1\boldsymbol{\rho}_2) \leq 1$$

with the upper limit being reached if and only if $\boldsymbol{\rho}_1 = \boldsymbol{\rho}_2$ is a pure state operator.

Proof.
Being a well defined inner product, the Hilbert–Schmidt inner product satisfies Schwartz inequality

$$\operatorname{Tr}(\boldsymbol{\rho}_1\boldsymbol{\rho}_2) \leq \sqrt{\operatorname{Tr}(\boldsymbol{\rho}_1^2)\operatorname{Tr}(\boldsymbol{\rho}_2^2)} \leq \sqrt{\operatorname{Tr}(\boldsymbol{\rho}_1)\operatorname{Tr}(\boldsymbol{\rho}_2)} \leq 1$$

The bound can be reached if $\boldsymbol{\rho}_1$, $\boldsymbol{\rho}_2$ are pure states. In such a case $\operatorname{Tr}(\boldsymbol{\rho}_1\boldsymbol{\rho}_2) = 1$ if and only if $\boldsymbol{\rho}_1 = \boldsymbol{\rho}_2$. □

Theorem. *A pure state cannot be expressed as a **non-trivial convex** combination of other states, but a non pure state can always be expressed in that way.*

Proof. Suppose that there exist a collection of $\wp_i > 0$ $i = 1, \dots, \mathscr{M}$ such that

$$\boldsymbol{\rho} = \sum_{i=1}^{\mathscr{M}} \wp_i\,\boldsymbol{\rho}_i \qquad \& \qquad \sum_{i=1}^{\mathscr{M}} \wp_i = 1$$

The Hilbert-Schmidt norm of the state is then

$$\|\boldsymbol{\rho}\|^2 = \sum_{i,j=1}^{\mathscr{M}} \wp_i\,\wp_j\,\operatorname{Tr}(\boldsymbol{\rho}_i\,\boldsymbol{\rho}_j)$$

By the previous proposition we then obtain the bound

$$\|\boldsymbol{\rho}\|^2 \leq \sum_{i,j=1}^{\mathscr{M}} \wp_i \, \wp_j = 1$$

As all the terms in the series are positive, the bound can be reached if and only if

$$\operatorname{Tr}(\boldsymbol{\rho}_i \, \boldsymbol{\rho}_j) = 1$$

for all i, j. But this means then

$$\boldsymbol{\rho} = \sum_{i=1}^{\mathscr{M}} \wp_i \, \boldsymbol{\rho}_1 = \boldsymbol{\rho}_1 \sum_{i=1}^{\mathscr{M}} \wp_i \; = \boldsymbol{\rho}_1$$

□

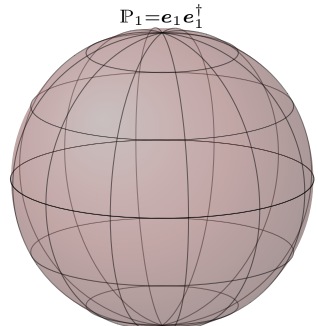
Pure states are points on the Bloch sphere

The geometrical content of the reseult proved above is most conveniently visualized in a two dimensional Hilbert space. In such a case, we can use spherical coordinates to map unit vectors on the sphere $\mathbb{S}^2$

$$\boldsymbol{f}_{\theta,\phi} = \cos\frac{\theta}{2}\boldsymbol{e}_1 + e^{\imath\phi}\sin\frac{\theta}{2}\,\boldsymbol{e}_2 \tag{7}$$

Correspondingly, we can think as well of pure states as point on the Bloch sphere

$$\boldsymbol{\rho}_{\theta,\phi} = \boldsymbol{f}_{\theta,\phi}\boldsymbol{f}^{\dagger}_{\theta,\phi} \tag{8}$$



The canonical basis of $\mathcal{M}_2(\mathbb{C})$ consists of outer products of among the elements of the canonical basis of $\mathbb{C}^2$

$$\mathbb{E}_{ij} = \boldsymbol{e}_i\boldsymbol{e}_j^{\dagger} \qquad i,j = 1,2$$

In the canonical basis the state operator (8) becomes

$$\boldsymbol{\rho}_{\theta,\phi} = \cos^2\frac{\theta}{2}\,\boldsymbol{e}_1\boldsymbol{e}_1^{\dagger} + \frac{1}{2}\sin\theta\left(e^{-\imath\phi}\boldsymbol{e}_1\boldsymbol{e}_2^{\dagger} + e^{\imath\phi}\boldsymbol{e}_2\boldsymbol{e}_1^{\dagger}\right) + \sin^2\frac{\theta}{2}\,\boldsymbol{e}_2\boldsymbol{e}_2^{\dagger}$$

In general, convenient way to choose a basis of $\mathcal{M}_d(\mathbb{C})$ is to take a set of self-adjoint matrices orthonormal with respect to the Hilbert-Schmidt inner product. A general strategy to construct such a basis is to complete the set of generators of the Lie algebra of the SU(d) group (see appendix for an explicit example of such construction and related references). For $d = 2$ this means

$$\mathbb{H}_0 = \frac{1}{\sqrt{2}}\mathbb{1}_2 \qquad \& \qquad \mathbb{H}_i = \frac{1}{\sqrt{2}}\sigma_i \quad i = 1,2,3$$

where the σ_i's stand for the Pauli matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \& \quad \sigma_2 = \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix} \quad \& \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

The choice of a self-adjoint orthonormal basis has the advantage that the coefficients of any self-adjoint matrix are then by construction real. For (8) we then get

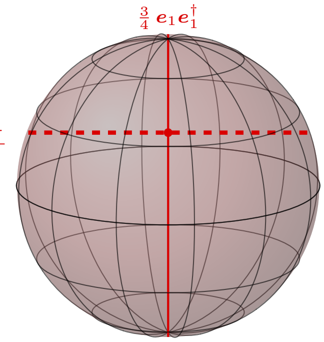
$$\boldsymbol{f}_{\theta,\phi}\boldsymbol{f}^{\dagger}_{\theta,\phi} = \frac{1}{2}\mathbb{1}_2 + \sin\theta\,(\cos\phi\,\sigma_1 + \sin\phi\,\sigma_2) + \cos\theta\,\sigma_3$$

Mixed states are points in the interior of the Bloch sphere

In general a state operator describes a mixture of the different pure states. The mixture is not unique, on the contrary a mixed state of any quantum system can be realized as an ensemble of pure states in an infinite number of different ways. A proof of this statement can be found in e.g. § 2.4.2 of [3]. We illustrate here the general case by again considering a two dimensional Hilbert space.

If there are only two pure states in the ensemble, then the density operator lies on the line joining their projectors. For instance, we may consider

$$\boldsymbol{\rho} = \frac{3}{4}\boldsymbol{e}_1\boldsymbol{e}_1^\dagger + \frac{1}{4}\boldsymbol{e}_2\boldsymbol{e}_2^\dagger \tag{9}$$



Recalling (7), we introduce the basis $\{\boldsymbol{f}_{\theta,0}, \boldsymbol{f}_{\theta,\pi}\}$ generically having non-orthogonal elements

$$\boldsymbol{f}^\dagger_{\theta,0}\boldsymbol{f}_{\theta,\pi} = \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = \cos\theta$$

If we now substitute

$$\boldsymbol{e}_1 = \frac{\boldsymbol{f}_{\theta,0} + \boldsymbol{f}_{\theta,\pi}}{2\,\cos\frac{\theta}{2}} \qquad \& \qquad \boldsymbol{e}_2 = \frac{\boldsymbol{f}_{\theta,0} - \boldsymbol{f}_{\theta,\pi}}{2\,\sin\frac{\theta}{2}}$$

into (9), we obtain

$$\begin{aligned}\boldsymbol{\rho} &= \frac{3}{4}\left(\frac{\boldsymbol{f}_{\theta,0} + \boldsymbol{f}_{\theta,\pi}}{2\,\cos\frac{\theta}{2}}\right)\left(\frac{\boldsymbol{f}_{\theta,0} + \boldsymbol{f}_{\theta,\pi}}{2\,\cos\frac{\theta}{2}}\right)^\dagger + \frac{1}{4}\left(\frac{\boldsymbol{f}_{\theta,0} - \boldsymbol{f}_{\theta,\pi}}{2\,\sin\frac{\theta}{2}}\right)\left(\frac{\boldsymbol{f}_{\theta,0} - \boldsymbol{f}_{\theta,\pi}}{2\,\sin\frac{\theta}{2}}\right)^\dagger \\ &= \left(\frac{3}{\cos^2\frac{\theta}{2}} + \frac{1}{\sin^2\frac{\theta}{2}}\right)\frac{\boldsymbol{f}_{\theta,0}\boldsymbol{f}^\dagger_{\theta,0}}{16} + \left(\frac{3}{\cos^2\frac{\theta}{2}} - \frac{1}{\sin^2\frac{\theta}{2}}\right)\frac{\boldsymbol{f}_{\theta,0}\boldsymbol{f}^\dagger_{\theta,\pi} + \boldsymbol{f}_{\theta,\pi}\boldsymbol{f}^\dagger_{\theta,0}}{16} + \left(\frac{3}{\cos^2\frac{\theta}{2}} + \frac{1}{\sin^2\frac{\theta}{2}}\right)\frac{\boldsymbol{f}_{\theta,\pi}\boldsymbol{f}^\dagger_{\theta,\pi}}{16}\end{aligned}$$

In particular, the choice

$$\cos\frac{\pi}{6} = \frac{\sqrt{3}}{2}$$

shows that we can write (9) as a mixture of a distinct pair of pure states

$$\boldsymbol{\rho} = \frac{\boldsymbol{f}_{\frac{\pi}{3},0}\boldsymbol{f}^\dagger_{\frac{\pi}{3},0}}{2} + \frac{\boldsymbol{f}_{\frac{\pi}{3},\pi}\boldsymbol{f}^\dagger_{\frac{\pi}{3},\pi}}{2}$$

Time evolution on and in the Bloch sphere

The Bloch sphere examples allows us also to visualize unitary evolution of pure and mixed states as well as the effect of a projective measurement. If the Hamiltonian is time independent, the solution of the Liouville-von Neumann equation reads in general

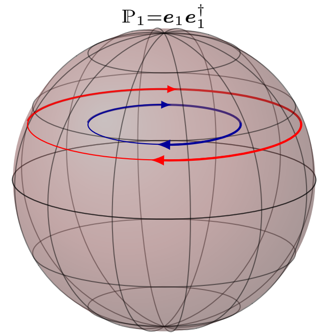
$$\boldsymbol{\rho}_t = \exp\left(-\imath\mathbb{H}t\right)\boldsymbol{\rho}_0\exp\left(\imath\mathbb{H}t\right)$$

For simplicity's sake we suppose

$$\mathbb{H}\boldsymbol{e}_i = (2 - i)\,E\,\boldsymbol{e}_i$$

Unitary evolution of a pure state, as to be expected, occurs on the surface of the Bloch sphere.

$$\exp(-\imath \mathbb{H} t)\, \boldsymbol{f}_{\theta,\phi} \boldsymbol{f}^{\dagger}_{\theta,\phi} \exp(\imath \mathbb{H} t) = \boldsymbol{f}_{\theta,\phi_t} \boldsymbol{f}^{\dagger}_{\theta,\phi_t}$$
$$\phi_t = \phi + E\, t$$



A projective measurement on the exited state $\mathbb{P}_1$ would produce a sudden collapse to the north pole. Finally, a mixed state with

$$\mathrm{Tr}\, \boldsymbol{\rho}_t^2 < 1$$

evolves in the interior of the Bloch sphere (Bloch ball).

APPENDIX

Self-adjoint basis for $\mathcal{M}_3(\mathbb{C})$

The basis consists of the identity matrix

$$\mathbb{H}_0 = \frac{1}{\sqrt{3}} \mathbb{1}_3$$

and the eight generators of the Lie algebra of SU(3) (see e.g. appendix A.1 of [1] for more details)

$$\mathbb{H}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \frac{\sigma_1 \oplus 0}{\sqrt{2}} \qquad \& \qquad \mathbb{H}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -\imath & 0 \\ \imath & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \frac{\sigma_2 \oplus 0}{\sqrt{2}}$$

$$\mathbb{H}_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \frac{\sigma_3 \oplus 0}{\sqrt{2}} \qquad \& \qquad \mathbb{H}_4 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

$$\mathbb{H}_5 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & -\imath \\ 0 & 0 & 0 \\ \imath & 0 & 0 \end{bmatrix} \qquad \& \qquad \mathbb{H}_6 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} = \frac{0 \oplus \sigma_1}{\sqrt{2}}$$

$$\mathbb{H}_7 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\imath \\ 0 & \imath & 0 \end{bmatrix} = \frac{0 \oplus \sigma_2}{\sqrt{2}} \qquad \& \qquad \mathbb{H}_8 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

* * *

[1] R. Alicki and K. Lendi. *Quantum Dynamical Semigroups and Applications*, volume 717 of *Lecture Notes in Physics*. Springer Berlin Heidelberg, 2007.

[2] I. Bengtsson and K. Zyczkowski. *Geometry of quantum states: an introduction to quantum entanglement*. Cambridge University Press, 2006.

[3] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, 10th anniversary edition edition, 2010.

[4] I. C. Percival. *Quantum State Diffusion*. Cambridge University Press, 2003.