

Quantum Measurement Formalism

(my notes on density operators and POVMs)

Fabio Grazioso
2015-06-23 17:49 (EST)

Contents

0.1 foreword	4
I part one: the quantum state	5
1 The quantum state - density operators	6
1.1 Introduction	6
1.2 Formal approach (Cohen-Tannoudji)	7
1.2.1 time dependence	7
1.3 Projector	8
1.4 Density operator	8
1.5 Density operator representing a mixture state	9
1.6 Matrix elements of the density matrices	9
1.6.1 diagonal elements	12
1.6.2 off diagonal elements	13
1.6.3 physical meaning of the off diagonal elements	13
1.6.4 Examples	14
1.6.5 pure states	14
1.6.6 mixed states	16
1.7 Expectation value	16
2 Algebraic approach	17
2.1 Hilbert space of pure states of a quantum system	17
2.1.1 Qualitative definition of pure states and mixed states	17
2.1.2 Operators on the states	18
2.2 Density operators	18
2.2.1 Definitions of trace, hermitianicity and positivity	19
2.2.2 Projectors are density operators	20
2.3 Projection operators	20
2.3.1 matrix representation	20
2.3.2 Properties of projectors	21
2.4 Linear combinations of projectors	21

2.5	Projector built with a pure state written as a superposition	23
2.6	projector built with a linear combination of pure states	24
2.6.1	Matrix representation	25
2.7	Summary of Pieter's introduction	25
2.8	Comments on coherent and incoherent superposition	26
2.9	Pieter's comments on superposition and evolution	27
2.10	Rank and purity	28
3	Mixed states of a qubit	29
3.1	Example of a density operators for the states in the BB84 protocol	29
3.1.1	Explicit density matrices	30
3.2	Bloch sphere: graphic representation	32
3.3	Visualizing the probabilities	34
II	Part two: the observable	35
4	Expectation values and probability of measurement outcomes	36
4.1	Expectation value of an observable, for a system in a pure state	36
4.2	Probability of the outcome of a measurement on a pure state	37
4.3	Expectation value of an observable, for a system in a mixture state	38
4.3.1	Probability of a measurement	38
4.3.2	Observable as function of the projectors on the eigenspaces	40
4.3.3	Expectation value of the observable	40
5	The observables - POVMs	43
5.1	General measurement, projective measurement and POVM	43
5.1.1	Projective measurement	43
5.1.2	General measurement	45
5.1.3	POVM	45
5.2	Example: the two POVMs of BB84	46
5.2.1	Example: POVMs of BB84 with passive choice	47
5.3	Example on [NC00] pag. 92	47
5.4	The Heisemberg indeterminacy principle	48
A		49
A.1	Sources of these notes	49

0.1 foreword

These notes are a collection of different material, coming from different times. In particular the notes on density operators and the notes on the POVMs were previously separate notes.

I am now doing an effort to combine all those notes in an organic account of the formalism to describe the quantum measurement process. (FG, Montreal, October 2012)

Part I

part one: the quantum state

Chapter 1

The quantum state - density operators

In this chapter: notes from dialogues with Rodolfo Figari, notes from Choen-Tannudji [CTDL05], and notes from dialogues with Frederich Grosshans.

1.1 Introduction

In general, the density operator formalism is useful to describe a quantum system of which we don't know the state, but we know a “set of *possible states*”, and the *probability distribution* of them.

In these notes I present several approaches:

- a description, more abstract, where the vectors and matrices are not written with an explicit representation in a specific basis (this is taken mostly from [CTDL05], and some dialogs with Rodolfo Figari).
- a description where the vectors and matrices are represented explicitly, in a chosen basis. This is taken from a dialogue with Pieter Kok. In this section will be discussed some algebraic properties of the density operators: projectors and linear combinations of projectors.
- an approach more specific to the Quantum Information Processing (taken from dialogues with Frederich Grosshans)

I also add some notes on the application to *entropy* computation.

1.2 Formal approach (Cohen-Tannoudji)

(see [CTDL05], complement E_{III} , vol I, page 295)

Let's consider the *normalized* quantum state $|\psi\rangle$, and let's write its expansion over the orthonormal basis states $\{|\varphi_n\rangle\}$:

$$|\psi\rangle = \sum_n c_n |\varphi_n\rangle \quad (1.1)$$

where the coefficients

$$c_n := \langle \varphi_n | \psi \rangle \quad (1.2a)$$

$$c_n^* := \langle \psi | \varphi_n \rangle \quad (1.2b)$$

satisfy the *normalization* condition:

$$\sum_n |c_n|^2 = 1. \quad (1.3)$$

Note: in general $\{|\varphi_n\rangle\}$ is not the eigenbasis of \hat{A} .

Let's consider the observable \hat{A} , and its matrix elements on the same orthonormal basis $\{|\varphi_n\rangle\}$:

$$A_{nm} = \langle \varphi_n | \hat{A} | \varphi_m \rangle. \quad (1.4)$$

The *mean value* of the observable \hat{A} on the state $|\psi\rangle$ is

$$\begin{aligned} \langle \hat{A} \rangle_\psi &= \langle \psi | \hat{A} | \psi \rangle \\ &= (\sum_n c_n^* \langle \varphi_n |) \hat{A} (\sum_m c_m | \varphi_m \rangle) \\ &= \sum_{n,m} c_n^* c_m A_{nm}. \end{aligned} \quad (1.5)$$

1.2.1 time dependence

If the state $|\psi\rangle$ is time dependent, its evolution is expressed by the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \quad (1.6)$$

and the mean value is

$$\langle \hat{A} \rangle_\psi(t) = \sum_{n,m} c_n^*(t) c_m(t) A_{nm} \quad (1.7)$$

where the time dependence is only in the coefficients, while the observable is constant (Schrödinger representation).

1.3 Projector

Since $c_n = \langle \varphi_n | \psi \rangle$, we can introduce the operator $\Pi_\phi \equiv |\phi\rangle\langle\phi|$ which is the *projection operator over the subspace* $|\psi\rangle$ (see formula D-36-a of [CTDL05], page 138), and see the quantities $c_m^* c_n$ as the matrix elements of the (matrix representation, in the $\{|\varphi_i\rangle\}$ basis, of the) operator Π_ϕ :

$$\begin{aligned} c_m^* c_n &= \langle \varphi_n | \psi \rangle \langle \psi | \varphi_m \rangle \\ &= \langle \varphi_n | \Pi_\phi | \varphi_m \rangle \\ &= (\Pi_\phi)_{nm} \end{aligned} \tag{1.8}$$

where it is important to notice the order of the indices! (check this on the book...)

1.4 Density operator

We want to give to the projector operator $\Pi_\phi \equiv |\phi\rangle\langle\phi|$ a broader meaning, so we say that it is a special case of a broader category of operators, called *density operators*, which we will indicate with $\hat{\rho}$. The density operators are defined by the following three properties:

- hermitian
- semi-positive definite
- trace = 1.

The relationship between the two types of operators is that

- all the projection operators are density operators
- some density operator are not projection operators.

In other words, the **density operators** are a broader category, which include the **projection operators**. It's possible to show that the density operators form a vector space, where the projection operators are the basis elements, and all the density operators which are not projectors, are linear combinations of projectors, with *real coefficients*.

Density operators can be associated to quantum states, i.e. they can *represent a quantum state*.

The *special case* of projectors are associated to **pure states**.

The general case of density operators which are **linear combinations of projectors**, are associated to **mixture states**.

For the density operators which are projectors we can rewrite the (1.8) as:

$$\begin{aligned} c_m^* c_n &= \langle \varphi_m | \psi \rangle \langle \psi | \varphi_n \rangle \\ &= \langle \varphi_m | \hat{\rho} | \varphi_n \rangle \\ &= [\hat{\rho}]_{nm} \end{aligned} \tag{1.9}$$

where it is important to notice the order of the indices! (see (1.8))

Finally, we observe that a time-dependent state is represented by a time-dependent density operator $\hat{\rho}(t)$.

1.5 Density operator representing a mixture state

A mixture state of a quantum system is one where we only know that the system can be in a set of some possible (pure) states $\{|\psi_1\rangle \dots |\psi_n\rangle\}$ with probabilities $\{p_1 \dots p_n\}$, where $\sum_k p_k = 1$.

We can then define a density operator representing this mixed state, as follows:

$$\begin{aligned} \hat{\rho} &:= \sum_k p_k |\psi_k\rangle \langle \psi_k| \\ &= \sum_k p_k \hat{\rho}_k. \end{aligned} \tag{1.10}$$

We observe that the trace of the density operator of the mixture is the “weighted sum” of the traces of the density operators of the pure states, the weights being the probabilities:

$$Tr(\hat{\rho}) = \sum_k p_k Tr(\hat{\rho}_k) \tag{1.11}$$

1.6 Matrix elements of the density matrices

Here we want to comment on the intuition and the “physical meaning” of the matrix elements of a density matrix. A density matrix is the representation, in a specific basis, of the *density operator*.

We will consider at first the case of a pure state, and then the case of a mixture state.

Let's consider a mixture state $|\psi\rangle$, with probability distribution $\{p_k\}$ and set of possible states $\{|\psi_k\rangle\}$ (pure states).

Let's also consider the basis $\{|\varphi_i\rangle\}$ of the hilbert space to which the pure states $\{|\psi_k\rangle\}$ belong.

We have seen that the density operator describing the pure state $|\psi_k\rangle$ is defined as:

$$\hat{\rho}_k := |\psi_k\rangle\langle\psi_k| \quad (1.12)$$

while the density operator describing the mixture state $|\psi\rangle$ is defined as:

$$\begin{aligned} \hat{\rho} &:= \sum_k p_k \hat{\rho}_k \\ &= \sum_k p_k |\psi_k\rangle\langle\psi_k|. \end{aligned} \quad (1.13)$$

Now, if we want to represent the density operators in the basis $\{|\varphi_i\rangle\}$, we first recall that a vector of the hilbert space is represented as:

$$\begin{aligned} |\psi_k\rangle &= \sum_i \langle\varphi_i|\psi_k\rangle |\varphi_i\rangle \\ &= \sum_i c_i^{(k)} |\varphi_i\rangle \end{aligned} \quad (1.14)$$

and

$$\begin{aligned} \langle\psi_k| &= \sum_i \langle\psi_k|\varphi_i\rangle \langle\varphi_i| \\ &= \sum_i c_i^{*(k)} \langle\varphi_i| \end{aligned} \quad (1.15)$$

with

$$\begin{cases} c_i := \langle\varphi_i|\psi\rangle \\ c_i^* := \langle\psi|\varphi_i\rangle. \end{cases} \quad (1.16)$$

In algebraic, matricial form:

$$\begin{aligned}
|\psi_k\rangle &= \begin{pmatrix} \langle\varphi_1|\psi_k\rangle \\ \langle\varphi_2|\psi_k\rangle \\ \dots \\ \langle\varphi_N|\psi_k\rangle \end{pmatrix} \\
&= \begin{pmatrix} c_1^{(k)} \\ c_2^{(k)} \\ \dots \\ c_N^{(k)} \end{pmatrix}
\end{aligned} \tag{1.17}$$

and

$$\begin{aligned}
\langle\psi_k| &= (\langle\psi_k|\varphi_1\rangle \quad \langle\psi_k|\varphi_2\rangle \quad \dots \quad \langle\psi_k|\varphi_N\rangle) \\
&= \left(c_1^{*(k)} \quad c_2^{*(k)} \quad \dots \quad c_N^{*(k)} \right)
\end{aligned} \tag{1.18}$$

where N is the dimension of the hilbert space (chosen finite for the sake of simplicity).

Then, the density matrix of the pure state will be:

$$\begin{aligned}
\hat{\rho}_k &= |\psi_k\rangle\langle\psi_k| \\
&= \begin{pmatrix} c_1^{(k)} \\ c_2^{(k)} \\ \dots \\ c_N^{(k)} \end{pmatrix} \cdot \left(c_1^{*(k)} \quad c_2^{*(k)} \quad \dots \quad c_N^{*(k)} \right) \\
&= \begin{pmatrix} c_1^{(k)} c_1^{*(k)} & c_1^{(k)} c_2^{*(k)} & \dots & c_1^{(k)} c_N^{*(k)} \\ c_2^{(k)} c_1^{*(k)} & c_2^{(k)} c_2^{*(k)} & \dots & c_2^{(k)} c_N^{*(k)} \\ \dots & \dots & \dots & \dots \\ c_N^{(k)} c_1^{*(k)} & c_N^{(k)} c_2^{*(k)} & \dots & c_N^{(k)} c_N^{*(k)} \end{pmatrix}.
\end{aligned} \tag{1.19}$$

The mixture state it will be

$$\begin{aligned}
\hat{\rho} &= \sum_k p_k \hat{\rho}_k \\
&= \sum_k p_k |\psi_k\rangle \langle \psi_k| \\
&= \sum_k p_k \left[\begin{pmatrix} c_1^{(k)} \\ c_2^{(k)} \\ \dots \\ c_N^{(k)} \end{pmatrix} \cdot \begin{pmatrix} c_1^{*(k)} & c_2^{*(k)} & \dots & c_N^{*(k)} \end{pmatrix} \right] \\
&= \sum_k p_k \left[\begin{pmatrix} c_1^{(k)} c_1^{*(k)} & c_1^{(k)} c_2^{*(k)} & \dots & c_1^{(k)} c_N^{*(k)} \\ c_2^{(k)} c_1^{*(k)} & c_2^{(k)} c_2^{*(k)} & \dots & c_2^{(k)} c_N^{*(k)} \\ \dots & \dots & \dots & \dots \\ c_N^{(k)} c_1^{*(k)} & c_N^{(k)} c_2^{*(k)} & \dots & c_N^{(k)} c_N^{*(k)} \end{pmatrix} \right] \\
&= \begin{pmatrix} \sum_k p_k c_1^{(k)} c_1^{*(k)} & \sum_k p_k c_1^{(k)} c_2^{*(k)} & \dots & \sum_k p_k c_1^{(k)} c_N^{*(k)} \\ \sum_k p_k c_2^{(k)} c_1^{*(k)} & \sum_k p_k c_2^{(k)} c_2^{*(k)} & \dots & \sum_k p_k c_2^{(k)} c_N^{*(k)} \\ \dots & \dots & \dots & \dots \\ \sum_k p_k c_N^{(k)} c_1^{*(k)} & \sum_k p_k c_N^{(k)} c_2^{*(k)} & \dots & \sum_k p_k c_N^{(k)} c_N^{*(k)} \end{pmatrix}.
\end{aligned} \tag{1.20}$$

1.6.1 diagonal elements

From (1.19) and (1.20) we can see how the diagonal elements of a pure state's density matrix are:

$$\begin{aligned}
[\hat{\rho}_k]_{ii} &= c_i^{(k)} c_i^{*(k)} \\
&= \langle \varphi_i | \psi_k \rangle \langle \psi_k | \varphi_i \rangle \\
&= |\langle \varphi_i | \psi_k \rangle|^2.
\end{aligned} \tag{1.21}$$

If the state is a mixture state, we have

$$\begin{aligned}
[\hat{\rho}]_{ii} &= \sum_k p_k [\hat{\rho}_k]_{ii} \\
&= \sum_k p_k c_i^{(k)} c_i^{*(k)} \\
&= \sum_k p_k \langle \varphi_i | \psi_k \rangle \langle \psi_k | \varphi_i \rangle \\
&= \sum_k p_k |\langle \varphi_i | \psi_k \rangle|^2.
\end{aligned} \tag{1.22}$$

If $\{|\varphi_i\rangle\}$ is the eigenbase of an observable, we can see how the diagonal elements of a density matrix represent the probabilities of the i -th eigenvalue to be the outcome of a measurement, given that the system is in $|\psi_k\rangle$ or in $\{|\psi_k\rangle$ respectively.

1.6.2 off diagonal elements

From (1.19) and (1.20) we can see how the **off-diagonal elements** of a pure state's density matrix are:

$$\begin{aligned} [\hat{\rho}_k]_{ij} &= c_i^{(k)} c_j^{*(k)} \\ &= \langle \varphi_i | \psi_k \rangle \langle \psi_k | \varphi_j \rangle. \end{aligned} \tag{1.23}$$

If the state is a mixture state, we have

$$\begin{aligned} [\hat{\rho}]_{ij} &= \sum_k p_k [\hat{\rho}_k]_{ij} \\ &= \sum_k p_k c_i^{(k)} c_j^{*(k)} \\ &= \sum_k p_k \langle \varphi_i | \psi_k \rangle \langle \psi_k | \varphi_j \rangle. \end{aligned} \tag{1.24}$$

1.6.3 physical meaning of the off diagonal elements

see [CTDL05, Complement E_{III} , §4c, pag 302] . See also [CTDL05, Chapter III, §E.1, pag 253]

This section has to be checked!

To give an intuitive physical meaning to the off-diagonal elements of a density operator linked to a mixture state, we see how they capture the concept of **quantum interference**.

In particular, if we consider a superposition of two quantum states, and we want to represent this **pure state** as a density matrix, in the off-diagonal terms the *interference terms* will appear.

Of course, the fact that a pure state is written as a superposition is a mere issue of *representation*, *i.e.* of the choice of the basis. So, a pure state in a basis in which it is written as a superposition, will be represented with a density matrix which is not diagonal, *i.e.* it will have **off-diagonal terms**.

On the other hand, if we consider an eigenstate, element of the basis chosen for the representation, its density matrix will be diagonal, and will have only a non zero term on the diagonal, which is equal to 1.

If we then consider the **mixed state** obtained combining two or more of such pure states, the corresponding density matrix will not have off-diagonal terms.

This shows again the difference between a mixed state and a superposition: only in the superposition (pure or mixed) the off-diagonal terms will appear.

So they are linked to the **quantum interference**, *i.e.* the phenomenon of the interference between **amplitudes of probability**.

As shown in [CTDL05, Chapter III, §E.1, pag 253], in formula (E-9), the probability of measuring the outcome linked to an eigenvalue contains the cross product of the projection of the two components of the superposition.

1.6.4 Examples

Let's consider the simplest case: an Hilbert space of dimension 2, which represents the state of a **qubit**:

$$\mathcal{H} := \text{span}\left\{|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\}. \quad (1.25)$$

The basis $\{|0\rangle, |1\rangle\}$ is known as the **computational basis**. We can also consider another basis, $\{|+\rangle, |-\rangle\}$, which is written in the computational basis representation in following way:

$$\begin{cases} |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \\ |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \end{cases} \quad (1.26)$$

1.6.5 pure states

The density operator representing the pure states $|0\rangle$ and $|1\rangle$ are respectively:

$$\rho_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 0) = \begin{pmatrix} (1 \cdot 1) & (1 \cdot 0) \\ (0 \cdot 1) & (0 \cdot 0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (1.27a)$$

$$\rho_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0, 1) = \begin{pmatrix} (0 \cdot 0) & (0 \cdot 1) \\ (1 \cdot 0) & (1 \cdot 1) \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.27b)$$

Since they are pure states, the diagonal terms are all 0 but one, which is 1. The rank is 1. Moreover, since they are represented in “their basis” (*i.e.* they are not superpositions), the off diagonal terms are zero.

On the other hand, in the computational basis the vectors (pure states) $|+\rangle$ and $|-\rangle$ are written as **superpositions**. So, the density operator representing $|+\rangle$ in the computa-

tional basis is :

$$\rho_+ = |+\rangle \langle +| \quad (1.28a)$$

$$= \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} [(|0\rangle + |1\rangle)(\langle 0| + \langle 1|)] \quad (1.28b)$$

$$= \frac{1}{2} \left\{ \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] \cdot [(1, 0) + (0, 1)] \right\} \quad (1.28c)$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 0) + \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0, 1) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1, 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0, 1) \right] \quad (1.28d)$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right] \quad (1.28e)$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad (1.28f)$$

$$= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad (1.28g)$$

For ρ_- we can use another (shorter) approach, and use the results in (1.26):

$$\rho_- = |-\rangle \langle -| \quad (1.29a)$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (1.29b)$$

$$= \begin{pmatrix} \left(\frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \right) & \left(-\frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \right) \\ \left(\frac{1}{\sqrt{2}} \cdot -\frac{1}{\sqrt{2}} \right) & \left(-\frac{1}{\sqrt{2}} \cdot -\frac{1}{\sqrt{2}} \right) \end{pmatrix} \quad (1.29c)$$

$$= \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad (1.29d)$$

Summarizing, **in the computational basis** the density operators for $|0\rangle$ and $|1\rangle$ are:

$$\begin{cases} \rho_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ \rho_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{cases} \quad (1.30)$$

while for $|+\rangle$ and $|-\rangle$ we have:

$$\begin{cases} \rho_+ = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \\ \rho_- = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \end{cases} \quad (1.31)$$

Notice how **all the four above states are pure states!**

(check if there is something to say about the **rank**).

1.6.6 mixed states

So, we have shown how the off diagonal terms appear when the state, in the basis chosen for the representation, is written as a superposition.

Let's now look at a **mixed state**. We want to write the density operator for the mixed state $\{\lambda_0 |0\rangle, \lambda_1 |1\rangle\}$ where $\lambda_{0,1} \in \mathbb{R}$ are probabilities, and therefore $\lambda_{0,1} \in [0, 1]$ and $\sum_{i \in \{0,1\}} \lambda_i = 1$. The density operator representing this mixture is:

$$\phi := \lambda_0 |0\rangle \langle 0| + \lambda_1 |1\rangle \langle 1| \tag{1.32a}$$

$$= \lambda_0 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \lambda_1 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.32b}$$

$$= \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \tag{1.32c}$$

Notice how the off-diagonal terms are 0 (no superposition). (check about the **rank**)

Now, let's consider a mixture state of $|+\rangle$ and $|-\rangle$:

$$\psi := \lambda_+ |+\rangle \langle +| + \lambda_- |-\rangle \langle -| \tag{1.33a}$$

$$= \lambda_+ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + \lambda_- \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{1.33b}$$

$$= \frac{1}{2} \begin{pmatrix} (\lambda_+ + \lambda_-) & (\lambda_+ - \lambda_-) \\ (\lambda_- - \lambda_+) & (\lambda_+ + \lambda_-) \end{pmatrix} \tag{1.33c}$$

$$= \begin{pmatrix} \frac{\lambda_+ + \lambda_-}{2} & \frac{\lambda_+ - \lambda_-}{2} \\ \frac{\lambda_- - \lambda_+}{2} & \frac{\lambda_+ + \lambda_-}{2} \end{pmatrix} \tag{1.33d}$$

1.7 Expectation value

see [CTDL05], complement E_{III} , page 300 and following

The expectation value for an observable \hat{A} measured on a mixed state ρ is given by

$$\langle \hat{A} \rangle_\rho = Tr(\rho \hat{A}) \tag{1.34}$$

(see formula 31 on page 301 of [CTDL05])

Chapter 2

Algebraic approach

In this chapter I report another possible introduction of the density operators, which is more abstract and algebraic, whereas the one from [CTDL05] is more centered on the explicit representation of the operators in a basis (matrices, with matrix element meanings).

This material is mainly based on discussions with Pieter Kok we had in Oxford in 2007.

2.1 Hilbert space of pure states of a quantum system

Let's start with a Hilbert space \mathcal{H} , which is the space of the states of our quantum system.

To make things easy let's say that \mathcal{H} has a finite dimension d . We can represent it's vectors as columns of d complex values.

Let's consider the following orthonormal basis:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \dots \tag{2.1}$$

2.1.1 Qualitative definition of pure states and mixed states

t ~ 57'

In the Copenhagen interpretation of quantum mechanics, in the state of the system there is all the possible information about the system. Then there are limits about how much of that information is accessible “at the same time” (Heisemberg indeterminacy).

But in line of principle, if the state of the system (i.e. one of it's representations, e.g. a wave function) is known, then everything about the system is “fixed”. A state contains the most complete knowledge about the system.

What we want to describe now, is how to represent a situation where we have only a partial information about the system.

The *pure states* are states with complete knowledge, and *mixed states* are the states with incomplete knowledge.

Let's consider two (pure) states of the system, i.e. two elements of the Hilbert space \mathcal{H} :

$$|\phi\rangle, |\psi\rangle \in \mathcal{H} \tag{2.2}$$

and let's suppose that we know that the system is in one of those two systems, but we don't know which. Let's say that we have two coefficients α and β that express the probability of being in the two states respectively, with $|\alpha|^2 + |\beta|^2 = 1$.

If we imagine to represent this situation with a superposition, this is wrong!

A superposition of the two states is a state:

$$|\Phi\rangle = \alpha|\phi\rangle + \beta|\psi\rangle, \tag{2.3}$$

again: this it is a state itself. To clarify this, consider that we could *change the basis* of the Hilbert space, and have a new representation where this state is no more a superposition.

So the superposition is not a suitable formalism to represent mixed states (incomplete knowledge).

Let's ask a question: what is about states that makes them states? One thing is that they are normalized: the different coefficients of a superposition sum up to 1 (mod squared), so that it is possible associate a probability to the coefficients.

2.1.2 Operators on the states

Let's consider the (linear) operators $\{A_k\}$ on the Hilbert space of the states:

$$A : |\phi\rangle \in \mathcal{H} \mapsto |\phi'\rangle \in \mathcal{H} \tag{2.4}$$

Those operators can be represented by $d \times d$ matrices.

2.2 Density operators

In this section we introduce the formal definition of *density operators*, as the operators $A : \mathcal{H} \mapsto \mathcal{H}$, which are *positive*, *hermitian*, and have *unitary trace*:

Definition 2.2.1 (Density operator)

$$\rho \text{ is a density operator} \Leftrightarrow \begin{cases} \rho \in \{A_k\} \\ \rho \text{ is positive} \\ \rho \text{ is hermitian} \\ \text{Tr } \rho = 1 \end{cases}$$

By now this is a formal definition. In what follows we will show a different, constructive approach to the density operators.

But now, in the next subsections we recall the definitions of the trace, and of positivity and hermiticity.

2.2.1 Definitions of trace, hermitianicity and positivity

Definition of trace

The *trace* of an operator can be defined as the sum of diagonal elements, since this sum is independent from the representation. As a corollary of this independence, the *trace* of A can be defined as the sum of its eigenvalues:

Definition 2.2.2 Trace

$$\text{Tr } A = \text{sum of eigenvalues}$$

Definition of hermitian operator

An hermitian operator is:

Definition 2.2.3 hermitian operator

$$A \text{ hermitian} \Leftrightarrow A = A^\dagger$$

This implies that their eigenvalues are real (this is a reason why physical observables are associated with hermitian operators).

Definition of positive operators

The property of the operator being “positive”, is that for each vector in \mathcal{H} , the expectation value of A on it is positive:

Definition 2.2.4 positive operator

$$A \text{ positive} \equiv \langle \phi | A | \phi \rangle \geq 0, \forall |\phi\rangle \in \mathcal{H}$$

2.2.2 Projectors are density operators

Theorem 2.2.1 *the projection operators are density operators*

2.3 Projection operators

We want now to introduce another definition of operators on \mathcal{H} , the *projection operators*. To do so, let's consider the *dual* of the Hilbert space \mathcal{H} , which we can call \mathcal{H}^D . In the bra-ket notation introduced by Dirac, we have $|\psi\rangle \in \mathcal{H}$ and $\langle\psi| \in \mathcal{H}^D$.

Definition 2.3.1 *Projector operator (or projector) - Given a vector $|\psi\rangle \in \mathcal{H}$ the projector operator associated to $|\psi\rangle$ is*

$$\Pi_\psi \equiv |\psi\rangle\langle\psi| \tag{2.5}$$

2.3.1 matrix representation

As an alternative to the Dirac notation, there is also a representation of the elements of \mathcal{H} and \mathcal{H}^D (states) as columns (of d elements), and rows respectively:

$$|\phi\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \in \mathcal{H} \tag{2.6}$$

$$\langle\phi| = (1, 0, 0, 0) \in \mathcal{H}^D \tag{2.7}$$

The inner product in this representation is a matrix product

$$\langle\phi|\phi\rangle = (1, 0, 0, 0) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 1. \tag{2.8}$$

Let's write a projection operator in this notation:

$$|\phi\rangle\langle\phi| = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} (1, 0, 0, 0) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv P_\phi \tag{2.9}$$

We could proof idempotence property directly, i.e. carrying out the product of the operator by itself in the matrix representation: $P_\phi^2 = P_\phi$.

2.3.2 Properties of projectors

We now introduce the property of an operator to be *idempotent*:

Definition 2.3.2 *idempotence an operator $A : \mathcal{H} \mapsto \mathcal{H}$ is idempotent iff*

$$A^2 = A \tag{2.10}$$

i.e.

$$\begin{aligned} A^2|\psi\rangle &= A(A|\psi\rangle) \\ &= A|\psi\rangle \end{aligned} \tag{2.11}$$

Theorem 2.3.1 *The projection operators are idempotent*

$$\begin{aligned} (|\phi\rangle\langle\phi|)^2 &= |\phi\rangle \underbrace{\langle\phi||\phi\rangle}_{1} \langle\phi| \\ &= |\phi\rangle \langle\phi|\phi\rangle \langle\phi| \\ &= |\phi\rangle 1 \langle\phi| \\ &= |\phi\rangle\langle\phi| \end{aligned} \tag{2.12}$$

Definition 2.3.3 *1D projector a projector is 1D iff it projects any state into a subspace spanned by a single state*

2.4 Linear combinations of projectors

We have associated each (pure) state of the system (each element of \mathcal{H}) with a 1D projection operator.

But the projection operators are represented by $d \times d$ matrices, so they span a space \mathcal{H}^2 that is bigger than the states space \mathcal{H} . Let's investigate the properties of this space, i.e. of it's elements.

In particular we want to study the “other” states, those relative to the *superpositions* of projectors.

Let's take two states (two elements of \mathcal{H})

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \tag{2.13}$$

and let's build with each of them a projector:

$$|\phi_1\rangle\langle\phi_1| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad |\phi_2\rangle\langle\phi_2| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.14}$$

Let's now consider the superposition of the two projectors. The coefficients of the superposition will be $p_1, p_2 \in [0, 1]; p_1 + p_2 = 1$, so that they can have the physical meaning of probabilities:

$$\begin{aligned}
\rho &= p_1|\phi_1\rangle\langle\phi_1| + p_2|\phi_2\rangle\langle\phi_2| \\
&= \begin{pmatrix} p_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned} \tag{2.15}$$

Theorem 2.4.1 *a linear combination of projectors is no more a projector,*
direct “proof”:

$$\begin{aligned}
\rho^2 &= \begin{pmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} p_1^2 & 0 & 0 \\ 0 & p_2^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \neq \rho.
\end{aligned} \tag{2.16}$$

Theorem 2.4.2 *any linear combination of projectors is a density operator*

Proof:

hermitianicity Let's recall that in general $(|a\rangle\langle b|)^\dagger = |b\rangle\langle a|$.

$$\rho^\dagger = p_1|\phi_1\rangle\langle\phi_1| + p_2|\phi_2\rangle\langle\phi_2| = \rho \Leftrightarrow \rho \text{ is hermitian} \tag{2.17}$$

positivity For all $|\psi\rangle \in \mathcal{H}$ we have:

$$\begin{aligned}
\langle\psi|\rho|\psi\rangle &= p_1\langle\psi|\phi_1\rangle\langle\phi_1|\psi\rangle + p_2\langle\psi|\phi_2\rangle\langle\phi_2|\psi\rangle \\
&= p_1|\langle\psi|\phi_1\rangle|^2 + p_2|\langle\psi|\phi_2\rangle|^2.
\end{aligned}$$

Since $p_1, p_2 \in \mathbb{R}^+$, we can conclude that

$$\forall|\psi\rangle \in \mathcal{H}, \quad \langle\psi|\rho|\psi\rangle \in \mathbb{R}^+ \stackrel{def}{\Leftrightarrow} \rho \text{ is positive.} \tag{2.18}$$

trace=1 Since we have chosen to build \mathcal{H}^2 with “normalized coefficients”, we have that

$$Tr \rho = p_1 + p_2 = 1. \tag{2.19}$$

2.5 Projector built with a pure state written as a superposition

Let's consider a state of \mathcal{H} which is written as a superposition (we use $\frac{1}{\sqrt{2}}$ as coefficient):

$$\frac{|\phi_1\rangle + |\phi_2\rangle}{\sqrt{2}}. \quad (2.20)$$

It is important to stress that this is a *pure state*, i.e. it is a single state of the \mathcal{H} space. In other words it is possible to find an observable such that this state is an eigenstate, so that the result of the measurement has no uncertainty.

The fact that a state is written as a superposition or not, only depends on the choice of the representation chosen.

To study this type of projectors, let's build one, i.e. let's build the projector operator based on the superposition state just introduced:

$$\begin{aligned} \rho' &\equiv \left(\frac{|\phi_1\rangle + |\phi_2\rangle}{\sqrt{2}} \right) \left(\frac{\langle\phi_1| + \langle\phi_2|}{\sqrt{2}} \right) \\ &= \frac{1}{2} (|\phi_1\rangle\langle\phi_1| + |\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|) \end{aligned}$$

If we use the column/row/matrix representation we can show that this element of \mathcal{H}^2 is a projector, i.e. that $\rho'^2 = \rho'$:

$$\begin{aligned} \rho' &= \frac{1}{2} (|\phi_1\rangle\langle\phi_1| + |\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|) \\ &= \frac{1}{2} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1, 0, 0) + \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (0, 1, 0) + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (1, 0, 0) + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0, 1, 0) \right] \\ &= \left[\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \\ &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

and, the square:

$$\begin{aligned}
\rho'^2 &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} \frac{1}{4} + \frac{1}{4} & \frac{1}{4} + \frac{1}{4} & 0 \\ \frac{1}{4} + \frac{1}{4} & \frac{1}{4} + \frac{1}{4} & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \rho'
\end{aligned}$$

2.6 projector built with a linear combination of pure states

Let's consider the two pure states:

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (2.21)$$

the third pure state, (coherent) superposition of the first two:

$$\frac{|\phi_1\rangle + |\phi_2\rangle}{\sqrt{2}} \quad (2.22)$$

the density operators built on the first two pure states (projectors):

$$|\phi_1\rangle\langle\phi_1| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad |\phi_2\rangle\langle\phi_2| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (2.23)$$

the density operator built on the third pure state (is a projection operator as well!):

$$\begin{aligned}
\rho' &\equiv \left(\frac{|\phi_1\rangle + |\phi_2\rangle}{\sqrt{2}} \right) \left(\frac{\langle\phi_1| + \langle\phi_2|}{\sqrt{2}} \right) \\
&= \frac{1}{2} (|\phi_1\rangle\langle\phi_1| + |\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|)
\end{aligned}$$

finally, the (incoherent) superposition of two density operators (this is a *density operator* which is not a *projection operator*!):

$$\rho = p_1|\phi_1\rangle\langle\phi_1| + p_2|\phi_2\rangle\langle\phi_2| \quad (2.24)$$

2.6.1 Matrix representation

If we look at the matrix representation of the *density operators*, depending on the choice of the basis they can have different representations.

But if we *diagonalize* the matrix we can tell whether we are dealing with a *density operator* which is a *projector* or just a *density operator*:

- the density operators which are projectors, have a representation matrix which in the diagonal form has just one non-zero element, which is equal to 1 (indeed, the trace must be 1)
- the other density operators (which are not projectors), have a representation matrix which in the diagonal form has more than one non-zero elements on the diagonal (which are ≤ 0 , since the trace must be zero).

2.7 Summary of Pieter's introduction

- we start with the hilbert space \mathcal{H} , of dimension d , called *pure states*. The states are represented as columns with d elements, and the basis is:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \dots \quad (2.25)$$

- we build the vector space \mathcal{H}^2 built using the elements $|\psi\rangle \in \mathcal{H}$ in the following way:
 - the basis elements of \mathcal{H}^2 are the *projection operators* $\Pi_\psi \equiv |\psi\rangle\langle\psi|$
 - then all the elements of \mathcal{H}^2 can be written as linear combinations of projection operators, with *real coefficients*
- It is possible to show that all the elements $\rho \in \mathcal{H}^2$ satisfy the following properties:

- a) ρ is hermitian
 - b) ρ is positive
 - c) $Tr \rho = 1$
- we call the operators $\rho \in \mathcal{H}^2$ (which all satisfy the three above properties) *density operators*
 - it is possible to show that a density operator $\rho \in \mathcal{H}^2$ which is a superposition of projection operators (with normalized, “probability” coefficients), it is not more a projector

We conclude that the space \mathcal{H}^2 of the density operators is divided in two groups:

- the density operators which are projectors
- the density operators which are not projectors

The first (projectors) are density operators built starting from an element $|\psi\rangle$ of \mathcal{H} as $\rho = |\psi\rangle\langle\psi|$, the second kind are spawned with superpositions of two or more of the first kind (with the real coefficients having the meaning of probabilities).

2.8 Comments on coherent and incoherent superposition

So far, we have meet the concept of superposition two times, in two different situations:

- projection operator built using a pure state which is written as a superposition
- linear combination (superposition) of two projection operators

so now we want to stress and investigate the difference.

We can re-phrase this in another way, in terms of “how to superimpose two pure states”. If we take two states $|\phi_1\rangle, |\phi_2\rangle \in \mathcal{H}$ we can think about two ways to superimpose them:

coherent we can **first** consider the state which is a superposition of the two, and **then** consider the density operator built with this state; in this way we will have a projection operator

incoherent we can **first** consider the two density operators built with the two states (two projection operators), and **then** consider the superposition of those two; in this way we will have a density operator which is not a projection operator.

In the first case, the coefficients of the superposition are complex numbers, so there will be a relative phase. In the second case the coefficients of the superposition are real, since they have the meaning of classical *probabilities*.

2.9 Pieter's comments on superposition and evolution

Let's consider two multi-particles systems, with a number n of the same particles, and let's consider n quantum states $\{\psi_1 \dots \psi_n\}$:

system A the particles are all in the same state, which is a superposition, with some real coefficients:

$$\sum_{i=1}^n c_i \psi_i \tag{2.26}$$

system B the particles are each in a quantum state, and the fraction of particles in each state is equal to the coefficient of the previous superposition.

To use the language of the previous subsection, system A is in a *coherent superposition*, system B is in a *incoherent superposition*.

If we measure an observable, the mean value of the measurement is the same for both systems. Nevertheless, there is a deep difference in the two systems. The difference is clear if we consider the evolution of both systems.

In the coherent superposition $|\psi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$, each particle “carries the phase” during the evolution, and therefore *interference phenomena* are possible. This is clear if we consider the modulus square of a superposition state, where the “cross terms” of the coefficients products are needed:

$$\begin{aligned} |\psi\rangle^2 &= |(c_1|\varphi_1\rangle + c_2|\varphi_2\rangle)|^2 \\ &= (c_1\langle\varphi_1| + c_2\langle\varphi_2|) (c_1|\varphi_1\rangle + c_2|\varphi_2\rangle) \\ &= c_1^2\langle\varphi_1|\varphi_1\rangle + c_1^*c_2\langle\varphi_1|\varphi_2\rangle + \\ &\quad + c_2^*c_1\langle\varphi_2|\varphi_1\rangle + c_2^2\langle\varphi_2|\varphi_2\rangle \end{aligned}$$

In the incoherent superposition the coefficients are “classical probabilities”, and the outcome is described by *conditional probability*.

Another example is a single particle passing a double slit. As long as we have no information about the path, both paths are possible, and so the state has to be described by a superposition of the two paths. Only in this description the interference can be described. In an incoherent superposition of several particles, no “classical probability” with real probability coefficients can give account of the interference!

2.10 Rank and purity

(from Patrick Hayden's class, lecture 10, $t \sim 35'45''$)

A density matrix representing a pure state is of rank 1. A density matrix representing a mixed state has rank > 1 .

Chapter 3

Mixed states of a qubit

In this chapter we focus on the mixed states of a quantum system which has only two pure states. This system is called *qubit* in the context of Quantum Information.

3.1 Example of a density operators for the states in the BB84 protocol

(see notes from [2011-10-03 rQKD-16](#))

(see also 2011-07-22)

In this section we give examples of how to compute density operators. We will compute the density operators describing the quantum state Eve measures, in few different situations.

In general, Eve receives a quantum state which is a mixture and not a pure state, since she only knows a set of possible states and their probability distribution.

Explicitly, if we call

$$\{|0\rangle, |1\rangle\} \tag{3.1}$$

the *computational basis*, and then we will have two more states, which form the *diagonal basis*

$$\{|+\rangle, |-\rangle\} = \left\{ \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \right\}. \tag{3.2}$$

Here is worth stressing that the *Hilbert space* of Alice's states has dimension 2, but the alphabet she uses has dimension 4. In other words we can relabel the alphabet in the

following way:

$$\begin{aligned}
|0\rangle &\rightarrow |0\rangle \\
|1\rangle &\rightarrow |1\rangle \\
|+\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \rightarrow |2\rangle \\
|-\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \rightarrow |3\rangle.
\end{aligned} \tag{3.3}$$

Two of the elements of the alphabet (two of the possible states) are linear combinations of the other two.

A possible confusion comes from forgetting that a state written as a superposition is a pure state. To this regard it is useful to consider that the fact that a state is written as a superposition or not, is merely a formal issue, due to the choice of the basis. Changing the basis, and switching from a representation which is a superposition to another which is not, does not change the physics of the system.

In the standard case where Eve receives the state from Alice with no further information (i.e. no information on the basis choice or on Bob's measurement), each possible state (each element of the alphabet) is equiprobable, so that the distribution of probability is

$$P(|i\rangle) = \frac{1}{4} \quad \forall |i\rangle \in \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}. \tag{3.4}$$

This mixed state is called *maximally mixed state*.

We can also consider other mixed states, where Eve has partial knowledge, so that the probability distribution is not constant.

For example we can have Eve's mixed state conditioned to the knowledge of Bob's measurement outcome.

If Eve knows that Bob's measurement outcome is $|0\rangle$, she knows the state cannot be $|1\rangle$ (here we are back to the computational basis notation). The probability distribution will be

$$\left\{\frac{1}{2}, 0, \frac{1}{4}, \frac{1}{4}\right\} \tag{3.5}$$

3.1.1 Explicit density matrices

To write the density matrices representing the mixture state Eve receives, we have to keep in mind that the Hilbert space these state belong to is two-dimensional, so the matrices will be 2×2 matrices. We can use as basis to represent the matrices the

computational basis. In this case, the pure state $|0\rangle$ is represented by

$$|0\rangle\langle 0| \quad (3.6a)$$

$$= \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 0) \quad (3.6b)$$

$$= \boxed{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}} \quad (3.6c)$$

and the pure state $|1\rangle$ is represented by

$$|1\rangle\langle 1| \quad (3.7a)$$

$$= \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0, 1) \quad (3.7b)$$

$$= \boxed{\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}}. \quad (3.7c)$$

On the other hand, the pure state $|+\rangle$ will be:

$$|+\rangle\langle +| \quad (3.8a)$$

$$= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \cdot \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|) = \quad (3.8b)$$

$$= \frac{1}{2}(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|) \quad (3.8c)$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (1, 0) + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (0, 1) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot (1, 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot (0, 1) \right] \quad (3.8d)$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right] \quad (3.8e)$$

$$= \boxed{\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}}. \quad (3.8f)$$

and the pure state $|-\rangle$ will be:

$$|-\rangle\langle -| = \quad (3.9a)$$

$$= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \cdot \frac{1}{\sqrt{2}}(\langle 0| - \langle 1|) = \quad (3.9b)$$

$$= \frac{1}{2}(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|) \quad (3.9c)$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (1, 0) - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (0, 1) - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot (1, 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot (0, 1) \right] \quad (3.9d)$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right] \quad (3.9e)$$

$$= \boxed{\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}}. \quad (3.9f)$$

Density matrix of the maximally mixed state

Once we have the representation of the pure states as density matrices, the mixed states are "simply" written as linear combinations of pure states.

So, for example, the maximally mixed state is

$$\frac{1}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| + \frac{1}{4}|+\rangle\langle +| + \frac{1}{4}|-\rangle\langle -| \quad (3.10)$$

$$= \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{4} \end{pmatrix} + \begin{pmatrix} \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} \end{pmatrix} + \begin{pmatrix} \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} \end{pmatrix} \quad (3.11)$$

$$= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad (3.12)$$

Density matrix of the mixed state knowing Bob's measurement

In this case, not all the possible states are equiprobable. If Eve knows that Bob's measurement outcome has been $|0\rangle$ then the mixed state is

$$\rho = \frac{1}{2}|0\rangle\langle 0| + 0|1\rangle\langle 1| + \frac{1}{4}|+\rangle\langle +| + \frac{1}{4}|-\rangle\langle -| \quad (3.13)$$

and then the density matrix representing this state in the computational basis is:

$$\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} \end{pmatrix} + \begin{pmatrix} \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} \end{pmatrix} \quad (3.14)$$

$$= \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} \quad (3.15)$$

3.2 Bloch sphere: graphic representation

see notes from:

2011-10-03 rQKD-16, t=23', page 2

2011-11-21 TbPBB84-04, t= 21' 50", IMG_0717.jpg

see also 2011-07-22

Another approach to the mixed state is the graphical approach, using the representation on the Bloch sphere.

If we use as basis the computational basis (3.1)

$$\{|0\rangle, |1\rangle\}$$

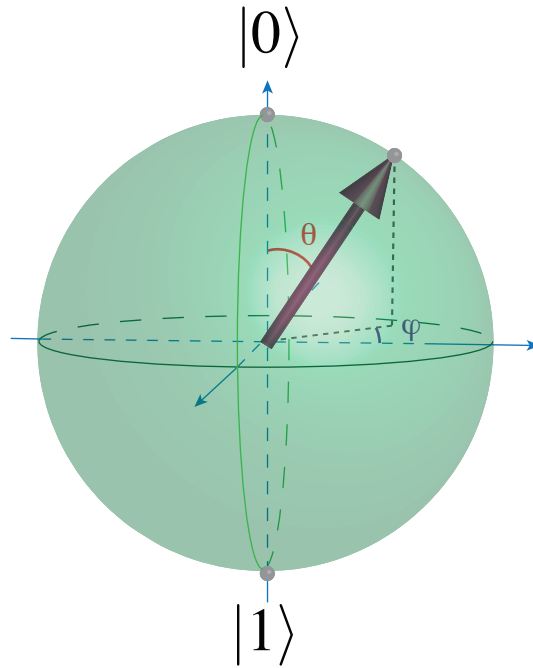


Figure 3.1: bloch sphere

The generic state is a linear combination of the two states $|0\rangle$ and $|1\rangle$ of the computational basis:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad (3.16)$$

At first, let's set $\varphi = 0$, i.e. let's consider only states along a "meridian" of the sphere. In this case the normalization condition is

$$|\alpha|^2 + |\beta|^2 = 1 \quad (3.17)$$

which, considering the trigonometric relation $\cos^2 * + \sin^2 * = 1$ can be written as

$$\begin{aligned} |\psi\rangle &= \cos * |0\rangle + \sin * |1\rangle \\ \alpha &= \cos * \\ \beta &= \sin * \end{aligned} \quad (3.18)$$

where $*$ is a suitable angle. Since we want to be $\theta \in [0, \pi]$ (see figure 3.1) and

$$\begin{cases} \theta = 0 \Rightarrow (\alpha = 1; \beta = 0) \\ \theta = \pi \Rightarrow (\alpha = 0; \beta = 1) \end{cases} \quad (3.19)$$

we choose $\ast = \frac{\theta}{2}$ which fulfills the requirements:

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle. \quad (3.20)$$

3.3 Visualizing the probabilities

The probabilities of measuring $|0\rangle$ and $|1\rangle$ can be “visualized” easily considering the projection on the vertical axis of the Bloch sphere, of the generic vector’s apex (see figure 3.2): the square of the distance from this point and $|1\rangle$ on the axis will be *proportional* to the probability of measuring $|0\rangle$, and similarly for $|0\rangle$:

$$\begin{aligned} p(0|\psi) &= 1 - \cos\theta = 2\sin^2\frac{\theta}{2} \\ p(1|\psi) &= 1 + \cos\theta = 2\cos^2\frac{\theta}{2} \end{aligned} \quad (3.21)$$

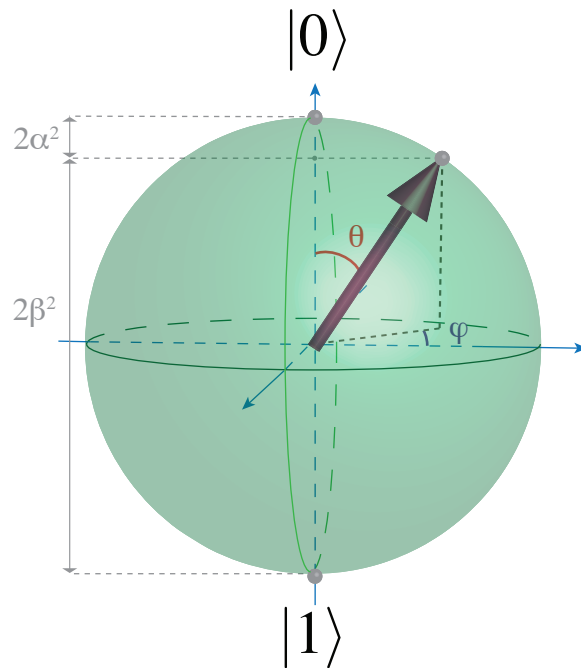


Figure 3.2: probabilities of a generic qubit state seen as (proportional to the) projections on the axis

To have the probabilities a renormalization is needed (total probability = 1)

Part II

Part two: the observable

Chapter 4

Expectation values and probability of measurement outcomes

This chapter continues from the approach from [CTDL05]. It has been postponed here because these notes are divided in two parts, so this fits more in this second part regarding the observables.

4.1 Expectation value of an observable, for a system in a pure state

One use of the density operator formalism is an alternative way of writing the expectation value of observables.

We are going to obtain an expression of the expectation value of the observable \hat{A} over the *pure* state $|\psi_k\rangle$ using two different “calculation strategies”. Here we use the index k for the pure state only as a link to the following: by now $|\psi_k\rangle$ is the only state the system is in, and is a pure state.

Let’s consider the *pure state* $|\psi\rangle$, and let’s rewrite the mean value of the observable \hat{A} (1.5) using the density operators:

$$\begin{aligned}\langle \hat{A} \rangle_\psi &= \langle \psi | \hat{A} | \psi \rangle \\ &= (\sum_n c_n^* \langle \varphi_n |) \hat{A} (\sum_m c_m | \varphi_m \rangle) \quad (\text{expanding } \psi \text{ as in (1.1)}) \\ &= \sum_{n,m} c_n^* c_m \langle \varphi_n | \hat{A} | \varphi_m \rangle \\ &= \sum_{n,m} c_n^* c_m A_{nm}\end{aligned}\tag{4.1}$$

This can be “visualized” if we explicitly write the states and the operator with vector and matrix representation in the basis $\{|\varphi_i\rangle\}$ in a case of dimension 3

$$\begin{aligned}
\langle\psi|\hat{A}|\psi\rangle &= \left(\langle\psi|\varphi_1\rangle \quad \langle\psi|\varphi_2\rangle \quad \langle\psi|\varphi_3\rangle \right) \begin{pmatrix} \langle\varphi_1|\hat{A}|\varphi_1\rangle & \langle\varphi_1|\hat{A}|\varphi_2\rangle & \langle\varphi_1|\hat{A}|\varphi_3\rangle \\ \langle\varphi_2|\hat{A}|\varphi_1\rangle & \langle\varphi_2|\hat{A}|\varphi_2\rangle & \langle\varphi_2|\hat{A}|\varphi_3\rangle \\ \langle\varphi_3|\hat{A}|\varphi_1\rangle & \langle\varphi_3|\hat{A}|\varphi_2\rangle & \langle\varphi_3|\hat{A}|\varphi_3\rangle \end{pmatrix} \begin{pmatrix} \langle\varphi_1|\psi\rangle \\ \langle\varphi_2|\psi\rangle \\ \langle\varphi_3|\psi\rangle \end{pmatrix} \\
&= \begin{pmatrix} c_1^* & c_2^* & c_3^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \\
&= \begin{pmatrix} c_1^* & c_2^* & c_3^* \end{pmatrix} \begin{pmatrix} A_{11}c_1 + A_{12}c_2 + A_{13}c_3 \\ A_{21}c_1 + A_{22}c_2 + A_{23}c_3 \\ A_{31}c_1 + A_{32}c_2 + A_{33}c_3 \end{pmatrix} \\
&= c_1^* \cdot (A_{11}c_1 + A_{12}c_2 + A_{13}c_3) + c_2^* \cdot (A_{21}c_1 + A_{22}c_2 + A_{23}c_3) + c_3^* \cdot (A_{31}c_1 + A_{32}c_2 + A_{33}c_3) \\
&= (A_{11}c_1^*c_1 + A_{12}c_1^*c_2 + A_{13}c_1^*c_3) + (A_{21}c_2^*c_1 + A_{22}c_2^*c_2 + A_{23}c_2^*c_3) + (A_{31}c_3^*c_1 + A_{32}c_3^*c_2 + A_{33}c_3^*c_3) \\
&= \sum_{n,m} c_n^* c_m A_{nm}
\end{aligned} \tag{4.2}$$

obtaining again the result in (4.1).

Now, using $A_{nm} = \langle\varphi_n|\hat{A}|\varphi_m\rangle$ and $[\hat{\rho}]_{nm} = c_m^* c_n$ as in (1.4) and (1.9):

$$\begin{aligned}
\langle\hat{A}\rangle_\psi &= \sum_{n,m} c_n^* c_m A_{nm} \\
&= \sum_{n,m} \langle\varphi_m|\hat{\rho}|\varphi_n\rangle \langle\varphi_n|\hat{A}|\varphi_m\rangle \\
&= \sum_m \langle\varphi_m|\hat{\rho}\hat{A}|\varphi_m\rangle \quad \left(\text{using } \sum_n |\varphi_n\rangle\langle\varphi_n| = 1 \right) \\
&= \sum_m [\hat{\rho}\hat{A}]_{mm} \\
&= Tr(\hat{\rho}\hat{A})
\end{aligned} \tag{4.3}$$

4.2 Probability of the outcome of a measurement on a pure state

Let's consider the probability that the outcome of the measurement of the observable \hat{A} gives as result the eigenvalue a_i given that the system is in the *pure* state $|\psi_k\rangle$. We comment that here we use the index k for the pure state only as a link to what follows:

by now $|\psi_k\rangle$ is the only state the system is in, and is a pure state. From the measurement postulate we know that:

$$\mathcal{P}(a_i|\psi_k) = |\langle a_i|\psi_k\rangle|^2. \quad (4.4)$$

We want to “expand” this writing, in order to express this in terms of the density operator $\hat{\rho}_k$ relative to the pure state $|\psi_k\rangle$:

$$\begin{aligned} \mathcal{P}(a_i|\psi_k) &= |\langle a_i|\psi_k\rangle|^2 \\ &= \langle \psi_k|a_i\rangle \langle a_i|\psi_k\rangle \\ &= \langle \psi_k|\hat{\Pi}_i|\psi_k\rangle \end{aligned} \quad (4.5)$$

where we have defined the **projector operator** relative to the eigenvector $|a_i\rangle$:

$$\hat{\Pi}_i := |a_i\rangle\langle a_i| \quad (4.6)$$

Once we have defined this operator, we can read the equation (4.5) as the *expectation value of the operator* $\hat{\Pi}_i$, and therefore we can apply the result of (4.3):

$$\mathcal{P}(a_i|\psi_k) = \text{Tr}(\hat{\rho}_k\hat{\Pi}_i) \quad (4.7)$$

4.3 Expectation value of an observable, for a system in a mixture state

We can use the density operator representing a mixture state to write the expectation value of an observable in a mixture state.

4.3.1 Probability of a measurement

Let’s consider an observable \hat{A} , and one of it’s eigenvalues a_i , with the associated (normalized) eigenstate $|a_i\rangle$.

Let’s also define the projector on the eigenstate $|a_i\rangle$ as

$$\hat{\Pi}_{a_i} \equiv |a_i\rangle\langle a_i| \quad (4.8)$$

conditional probability

The *conditional probability* $\mathcal{P}(a_i|\psi_k)$ that a measurement of \hat{A} yields as result a_i given that the state of the system is in the pure state $|\psi_k\rangle$ is

$$\mathcal{P}(a_i|\psi_k) = |\langle a_i|\psi_k\rangle|^2. \quad (4.9)$$

Using the projector (4.8) we can rewrite the *conditional probability* of the outcome as:

$$\begin{aligned} \mathcal{P}(a_i|\psi_k) &= |\langle a_i|\psi_k\rangle|^2 \\ &= (\langle a_i|\psi_k\rangle)^* \cdot (\langle a_i|\psi_k\rangle) \\ &= \langle \psi_k|a_i\rangle \langle a_i|\psi_k\rangle \\ &= \langle \psi_k|\hat{\Pi}_{a_i}|\psi_k\rangle. \end{aligned} \quad (4.10)$$

Now, we notice that this is in the form of the expectation value of an operator on a (pure) state, so we want to express it in terms of the density operator of the state, in analogy with (4.3):

$$\begin{aligned} \mathcal{P}(a_i|\psi_k) &= \langle \psi_k|\hat{\Pi}_{a_i}|\psi_k\rangle \\ &= (\sum_l \langle \varphi_l|c_l^{*(k)}\rangle) \hat{\Pi}_{a_i} (\sum_j c_j^{(k)}|\varphi_j\rangle) \\ &= \sum_{l,j} c_l^{*(k)} c_j^{(k)} \langle \varphi_l|\hat{\Pi}_{a_i}|\varphi_j\rangle \\ &= \sum_{l,j} c_l^{*(k)} c_j^{(k)} [\hat{\Pi}_{a_i}]_{lj} \end{aligned} \quad (4.11)$$

now we use the definition of (matrix elements of) the density operator of the state $|\psi_k\rangle$

$$c_l^{*(k)} c_j^{(k)} = [\hat{\rho}_k]_{jl}$$

and then

$$\begin{aligned} \mathcal{P}(a_i|\psi_k) &= \sum_{lj} [\hat{\rho}_k]_{lj} [\hat{\Pi}_{a_i}]_{lj} \\ &= \sum_{lj} \langle \varphi_j|\hat{\rho}_k|\varphi_l\rangle \langle \varphi_l|\hat{\Pi}_{a_i}|\varphi_j\rangle \quad (\text{using } \sum_l |\varphi_l\rangle \langle \varphi_l| = 1) \\ &= \sum_j \langle \varphi_j|\hat{\rho}_k \hat{\Pi}_{a_i}|\varphi_j\rangle \\ &= \text{Tr}(\hat{\rho}_k \hat{\Pi}_{a_i}) \end{aligned} \quad (4.12)$$

marginal probability

Now we look for the *marginal probability* $\mathcal{P}(a_i)$ of the result a_i if we measure the observable \hat{A} and we know the system is in the mixture state $\{|\psi_1\rangle \dots |\psi_n\rangle\}$. The marginal probability is obtained as a summation of the conditional probabilities of each stat, each “weighted” with the probability of each state $|\psi_k\rangle$:

$$\mathcal{P}(a_i) = \sum_k p_k \mathcal{P}(a_i|\psi_k) \quad (4.13)$$

then, using (4.12) we can express the probabilities $\mathcal{P}(a_i|\psi_k)$ in terms of the density operators of the pure states :

$$\mathcal{P}(a_i) = \sum_k p_k \text{Tr}(\hat{\rho}_k \hat{\Pi}_i) \quad (4.14)$$

4.3.2 Observable as function of the projectors on the eigenspaces

Before writing the expectation value of the observable \hat{A} on the mixture state $\{|\psi_k\rangle\}$ as function of the density operator representing the mixture, we have to recall the following:

it is possible to write the hermitian operator \hat{A} as linear combination of the projectors on his eigenspaces, with the eigenvalues as coefficients:

$$\begin{aligned} \hat{A} &= \sum_i a_i \hat{\Pi}_i \\ &= \sum_i a_i |a_i\rangle \langle a_i| \end{aligned} \quad (4.15)$$

4.3.3 Expectation value of the observable

Let's now calculate the expectation value of the observable \hat{A} if the state of the system is the mixture state $\{|\psi_k\rangle\}$, with probability distribution $\{p_k\}$.

In general the expectation value can be written as the sum of all the possible results (eigenvalues) weighted with their (marginal) probability $\mathcal{P}(a_i)$ (marginal probability for the outcome a_i of the measurement, i.e. summed over all the possible states of the system):

$$\langle \hat{A} \rangle_{\{|\psi_k\rangle\}} = \sum_i a_i \mathcal{P}(a_i) \quad (4.16)$$

In (4.14) we have seen how to express the (marginal) probability $\mathcal{P}(a_i)$, in the case of a mixture state, as function of the density operator which describes the state. So we substitute, obtaining:

$$\begin{aligned}
\langle \hat{A} \rangle_{\{|\psi_k\rangle\}} &= \sum_i a_i \left[\sum_k p_k \text{Tr}(\hat{\rho}_k \hat{\Pi}_i) \right] \\
&= \sum_i a_i \left[\text{Tr} \left(\sum_k p_k \hat{\rho}_k \hat{\Pi}_i \right) \right] \\
&= \sum_i a_i \left[\text{Tr} \left(\hat{\rho} \hat{\Pi}_i \right) \right] \\
&= \text{Tr} \left(\sum_i a_i \hat{\rho} \hat{\Pi}_i \right) \\
&= \text{Tr} \left(\hat{\rho} \sum_i a_i \hat{\Pi}_i \right)
\end{aligned} \tag{4.17}$$

now we consider the “expansion” of the operator \hat{A} on the set of the projectors on its eigenspaces $\hat{A} = \sum_i a_i \hat{\Pi}_i$, and so we can rewrite:

$$\langle \hat{A} \rangle_{\{|\psi_k\rangle\}} = \text{Tr} \left(\hat{\rho} \hat{A} \right). \tag{4.18}$$

In this way we have re-obtained, also in this case of a mixed state, the same result (4.3) seen in the case of a pure state.

expectation value of a superposition state (interference)

cfr chap III, §E, [CTDL05], page 252

Let's consider two orthonormal vectors of the Hilbert space:

$$\{|\psi_1\rangle, |\psi_2\rangle\} \tag{4.19}$$

we can think at them as two eigenvalues of an operator \hat{B} .

Let's now consider the state

$$|\psi\rangle = \lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle \tag{4.20}$$

which is a *linear superposition* of the states (4.19). Let's suppose that $|\psi\rangle$ is normalized, i.e. $\lambda_1 + \lambda_2 = 1$.

The whole point of this subsection is to stress the fact that $|\psi\rangle$ is a pure state, and not a mixture, even the λ are normalized.

Let's now consider an observable \hat{A} , with eigenstates $\{|a_i\rangle\}_i$ and corresponding eigenvalues $\{a_i\}_i$

We want to calculate the probability $P(a_i|\psi)$ that a measure of \hat{A} returns the eigenvalue a_i .

Following the measurement postulate (Born's rule), we write this probability as the square modulus of the projection of the state onto the corresponding eigenstate:

$$\begin{aligned}
 P(a_i|\psi) &= |\langle a_i|\psi\rangle|^2 \\
 &= |\langle a_i|(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle)|^2 \\
 &= |\lambda_1\langle a_i|\psi_1\rangle + \lambda_2\langle a_i|\psi_2\rangle|^2 \\
 &= (\lambda_1^*\langle\psi_1|a_i\rangle + \lambda_2^*\langle\psi_2|a_i\rangle)(\lambda_1\langle a_i|\psi_1\rangle + \lambda_2\langle a_i|\psi_2\rangle) \\
 &= (\lambda_1^*\langle\psi_1|a_i\rangle + \lambda_2^*\langle\psi_2|a_i\rangle)(\lambda_1\langle a_i|\psi_1\rangle + \lambda_2\langle a_i|\psi_2\rangle)
 \end{aligned} \tag{4.21}$$

Chapter 5

The observables - POVMs

(see:

2011-12-15 TbPBB84-07

2012-01-13 TbPBB84-14, 1h 20' 50", img_1613)

This chapter is based mainly on discussions with Frederic Grosshans in Paris, in 2012, and on [\[NC00\]](#)

5.1 General measurement, projective measurement and POVM

In the introductory formulation of quantum mechanics, the measurement postulate is introduced mentioning “the operator associated with an observable”, which is an hermitian operator.

This is a rather simplistic description, with respect to what is needed for quantum information theory (see e.g. [\[NC00\]](#)), so here we are going to different descriptions that are each more general than the previous.

5.1.1 Projective measurement

The first type of measurement we describe is the *projective measurement*, or *von Neumann measurement*, and is the closest to the description given in the introductory courses. In this case the measurement is represented by an operator \hat{M} such that:

$$\hat{M} = \sum_m m \hat{P}_m \tag{5.1}$$

where the $\{m\}$, the eigenvalues of \hat{M} , are the possible outcomes of the measurement, and $\{\hat{P}_m\}$ are the *orthogonal projectors* on the corresponding eigenspaces. The properties of

projectors are:

$$\forall m, \hat{P}_m \text{ is hermitian} \quad (5.2a)$$

$$\forall m, m', \hat{P}_m \hat{P}_{m'} = \delta_{m,m'} \hat{P}_m. \quad (5.2b)$$

The probability that the outcome of the measurement is m when the system is in the state $|\psi\rangle$ is:

$$p_\psi(m) = \langle \psi | \hat{P}_m | \psi \rangle; \quad (5.3)$$

and soon after such measurement the state of the system is:

$$\frac{\hat{P}_m |\psi\rangle}{\sqrt{p_\psi(m)}}. \quad (5.4)$$

From the requirement that the sum of all the probabilities (5.3) is equal to one we have the property of *completeness* for the set of projectors:

$$\sum_m \hat{P}_m = \mathbb{I}. \quad (5.5)$$

The expectation value of the measurement \hat{M} if the system is in the state $|\psi\rangle$ is:

$$\begin{aligned} E_\psi(\hat{M}) &= \sum_m m p_\psi(m) \\ &= \sum_m m \langle \psi | P_m | \psi \rangle \\ &= \langle \psi | \left(\sum_m m P_m \right) | \psi \rangle \\ &= \langle \psi | \hat{M} | \psi \rangle \\ &= \langle \hat{M} \rangle_\psi \end{aligned} \quad (5.6)$$

and the standard deviation is:

$$\begin{aligned} \Delta(\hat{M}) &= \sqrt{\langle (\hat{M} - \langle \hat{M} \rangle_\psi)^2 \rangle_\psi} \\ &= \sqrt{\langle \hat{M}^2 \rangle_\psi - \langle \hat{M} \rangle_\psi^2} \end{aligned} \quad (5.7)$$

where we have used the compact notation $\langle \psi | \cdot | \psi \rangle = \langle \cdot \rangle_\psi$.

5.1.2 General measurement

A second type of measurement is the *general measurement*, which is a generalization of the projective measurement. The general measurement is represented by a set of operators $\{\hat{M}_m\}$, called *Krauss operators*.

If we define:

$$\hat{P}_m = \hat{M}_m^\dagger \hat{M}_m, \quad (5.8)$$

we can use for the general measurement the same definitions of probability of an outcome, state of the system after a measurement, and the property of completeness, expressed by the equations (5.1) - (5.5), rewritten in terms of the Krauss operators. However, the difference with the projective measurement is that for the general measurement the $\{\hat{P}_m\}$ are in general not *projectors*.

5.1.3 POVM

Finally, it is possible to generalize the projective measurement and define the POVM (positive operator-valued measurement, see e.g. [NC00]), where some of the hypotheses of the projective measurement are relaxed. In this case, to represent the measurement we consider the set of operators:

$$\{\hat{E}_m\}. \quad (5.9)$$

Similarly to the projective measurement, the probability that the outcome is m if the system is in $|\psi\rangle$ is:

$$p_\psi(m) = \langle \psi | \hat{E}_m | \psi \rangle \quad (5.10)$$

with the property of completeness: $\sum_m \hat{E}_m = \hat{\mathbb{I}}$. But as for the general measurement, since operators (5.9) are not in general projectors, in general we can not write the $\{\hat{E}_m\}$ in terms of the Krauss operators, as in (5.8). An important consequence of this is that for the POVM measurement it is not defined the state of the system *after the measurement*. A common situation with POVM measurement is when we have a quantum system in a mixed state, where the set of possible states are represented by some vectors of the Hilbert space $\{|\psi_m\rangle\}$, not necessarily orthogonal to each other, and we want a measurement in order *to know in which of the states of the set the system is*. This POVM is represented by the set of operators:

$$\{\hat{E}_m = |\psi_m\rangle \langle \psi_m|\}. \quad (5.11)$$

These last operators are indeed projectors; however, since the $\{|\psi_m\rangle\}$ are not necessarily orthogonal, this POVM *is not* in general a projective measurement. In this type of

POVM, since the set of states does not necessarily form a basis of the Hilbert space, the completeness property has in general to be guaranteed with suitable normalization coefficients.

For more details see also [NC00] postulate 3 on page 84, beginning of page 88 and box 2.5 on page 91.

5.2 Example: the two POVMs of BB84

The Hilbert space is the qubit space, i.e. a two dimensional space. In this space we can perform two distinct measurements, based on two bases we choose, the *computational basis*:

$$\{|0\rangle, |1\rangle\} \tag{5.12}$$

and the *diagonal basis*:

$$\{|+\rangle, |-\rangle\} \tag{5.13}$$

where:

$$\begin{cases} |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \end{cases} \tag{5.14}$$

Let's build the explicit matrices representing the two POVM. We will represent the matrices in the computational basis. The first POVM, i.e. the measurement “in the computational basis”, has two outcomes, i.e. two elements. The first element is “measuring” the $|0\rangle$ state, and is represented by

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{5.15}$$

and the second is “measuring” the $|1\rangle$ state, and is represented by

$$|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.16}$$

About the measurement “in the diagonal basis”, the first POVM \hat{B}_{X-} is built as the

projector on the $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ in the following way

$$|+\rangle\langle+| \tag{5.17a}$$

$$= \frac{1}{2}(|0\rangle - |1\rangle)(\langle 0| - \langle 1|) \tag{5.17b}$$

$$= \frac{1}{2}(|0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|) \tag{5.17c}$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 & \\ & 0 \end{pmatrix} (1, 0) - \begin{pmatrix} 1 & \\ & 0 \end{pmatrix} (0, 1) - \begin{pmatrix} 0 & \\ & 1 \end{pmatrix} (1, 0) + \begin{pmatrix} 0 & \\ & 1 \end{pmatrix} (0, 1) \right] \tag{5.17d}$$

$$= \frac{1}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right] \tag{5.17e}$$

$$= \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{5.17f}$$

Similarly, the POVM element linked to $|+\rangle$ is:

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{5.18}$$

5.2.1 Example: POVMs of BB84 with passive choice

If the choice of the basis is done randomly by the apparatus itself (e.g. using a supplementary 50/50 beam splitter), we have a single POVM, made of four elements: the same four POVMs seen above for the “active choice” case, multiplied by a supplementary $\frac{1}{2}$ coefficient due to the “basis choice”. The POVMs are then equal to:

$$\left\{ \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} \end{pmatrix}, \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix} \right\} \tag{5.19}$$

5.3 Example on [NC00] pag. 92

In this example we have a set of possible quantum states which are not orthogonal. On the other hand, we have a POVM which is built “ad hoc” to be able to do an *unambiguous discrimination*, i.e. a measurement where in some cases the outcome allows to be sure about the state, but in some cases does not, but giving always the information of which case we are in.

The state are:

$$|\psi_1\rangle = |0\rangle \tag{5.20a}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{5.20b}$$

and the POVM elements are:

$$\hat{E}_1 = \frac{\sqrt{2}}{1 + \sqrt{2}} |1\rangle\langle 1| \quad (5.21a)$$

$$\hat{E}_2 = \frac{\sqrt{2}}{1 + \sqrt{2}} \frac{(|0\rangle - |1\rangle)(\langle 0| - \langle 1|)}{2} \quad (5.21b)$$

$$\hat{E}_3 = \mathbb{I} - \hat{E}_1 - \hat{E}_2 \quad (5.21c)$$

It is easy to show, by direct calculation, that:

$$\langle \psi_1 | \hat{E}_1 | \psi_1 \rangle = 0 \quad (5.22a)$$

$$\langle \psi_2 | \hat{E}_2 | \psi_2 \rangle = 0 \quad (5.22b)$$

so, if the outcome is E_1 or E_2 , we know the state of the system. If the outcome is E_3 we have an ambiguous outcome.

Note: here I am not sure of the reason or the physical meaning of the coefficients. It can not be because of the completeness ($\sum_i \hat{E}_i = \hat{\mathbb{I}}$), because the completeness is “automatic” with the definition of \hat{E}_3 .

5.4 The Heisemberg indeterminacy principle

Starting from [equation \(5.7\)](#) it is possible to introduce in an elegant way the *indeterminacy principle* (see [\[NC00\]](#) box 2.4, page 89).

Appendix A

A.1 Sources of these notes

- Sections from 2.1 to 2.7 are an account of Pieter Kok's notes (Oxford, 6/6/2007).
- Section 2.9 and 1.2 are from notes by Rodolfo Figari (Capri, aug 2005) and from [\[CTDL05\]](#)

Bibliography

- [CTDL05] Claude Cohen-Tannoudji, Bernard Diu, and Frank Laloe. *Quantum Mechanics (vol.1)*, volume 1. WILEY-VCH, wiley-vch edition, 2005.
- [NC00] Michael A. Nielsen and Isaac L. Chuang. Quantum information and computation. *Quantum Information and Computation*, 2000.

Index

density matrix, 9
density operators, 8
Kraus operators, 43
POVMs, 43
qubit, 29