Lecture May 13. Quantum.

(This notes are taken from the PhD thesis of Carlos Gonzalez-Guillen)

First, we fix the notation. Then, in Section 1 we present a short introduction to the mathematical formalism of quantum mechanics.

Through out this lecture we will be working with complex separable Hilbert spaces, we assume the reader is familiar with the basic knowledge and we just introduce the notation and terminology we are going to use.

- $\langle \varphi |$ is the dual vector of $|\varphi \rangle$ (conjugate transposed). Also known as bra.
- $\langle \varphi | \psi \rangle$ is the scalar product between $|\varphi \rangle$ and $|\psi \rangle$.
- $|\varphi \rangle |\psi \rangle$ or $|\varphi \rangle \otimes |\psi \rangle$ is the tensor product of $|\varphi \rangle$ and $|\psi \rangle$.
- $A^\dagger$ is the conjugate transposed or adjoint operator of $A$.
- $\langle \varphi | A | \psi \rangle$ is the scalar product between $|\varphi \rangle$ and $A|\psi \rangle$ or, equivalently, the scalar product between $A^\dagger|\varphi \rangle$ and $|\psi \rangle$.
- $|\varphi \rangle \langle \psi |$ is the outer product between $|\varphi \rangle$ and $|\psi \rangle$.

Given a pair of Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ we will denote as $B(\mathcal{H}_1, \mathcal{H}_2)$ the set of bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$. We will write $B(\mathcal{H}) := B(\mathcal{H}, \mathcal{H})$.

Let $\rho \in B(\mathcal{H})$ and $p \in [1, \infty)$, we denote as $\|\rho\|_p := \sqrt[p]{\sum_i \sigma_i^p}$ the Schatten $p$-norm of $\rho$, where $\sigma_i$ are the singular values of $\rho$. Thus $\|\rho\|_1 = \text{tr} \sqrt{\rho^\dagger \rho}$ is the trace norm of $\rho$, $\|\cdot\|_2$ is the Hilbert-Schmidt norm and $\|\rho\|_\infty := \max \sigma_i$ is the operator norm. The trace distance between two operators $\rho, \sigma \in B(\mathcal{H})$ is given by $\Delta(\rho, \sigma) := \frac{1}{2} \|\rho - \sigma\|_1$.

**Definition 0.1.** A density operator (or density matrix) $\rho \in B(\mathcal{H})$ is a non-negative self adjoint operator with unit trace, that is, $\rho \geq 0$ and $\text{tr} \rho = 1$. A density operator $\rho$ of rank one is called pure state. Otherwise, we say that
\( \rho \) is a mixed state. We denote by \( D_1(\mathcal{H}) \) the set of density operators of a Hilbert space \( \mathcal{H} \).

The condition \( \text{tr} \\rho = 1 \) is known as the normalization condition. We will identify a positive operator with an unnormalized density operator. For pure states we can write \( \rho = |\varphi\rangle \langle \varphi| \) where the normalization translates in \( |\varphi\rangle \) being a unit vector of \( \mathcal{H} \). In this case we will identify \( \rho \) and \( |\varphi\rangle \) and we will refer to both representations as pure states. The vector \( |\varphi\rangle \) is unique up to multiplication by a phase (a complex number of modulus one) \( e^{i\theta} \). Thus, any two pure states that differs in a phase have the same density matrix and hence represent the same state vector. Equality of vectors representing pure states should be understood in this sense. Nevertheless, whenever we want to highlight this fact, we will write \( |\varphi\rangle \equiv |\psi\rangle \) if \( |\varphi\rangle \) and \( |\psi\rangle \) represent the same state. That is, they differ in a phase or, if they are not normalized, they are equal up to a complex number.

Mixed states can also be diagonalised \( \rho = \sum_i p_i |\varphi_i\rangle \langle \varphi_i| \), where \( \sum_i p_i = 1 \) and \( |\varphi_i\rangle \) is a unit vector of \( \mathcal{H} \) for all \( i \). In this case, one usually refer to \( \rho \) as an (statistical) ensemble of pure states \( \{p_i, |\varphi_i\rangle\} \).

Positive maps between operators of Hilbert spaces take positive operators to positive operators. Moreover, a map \( T : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}') \) is completely positive if the map \( T \otimes 1_n : \mathcal{B}(\mathcal{H}) \otimes \mathcal{M}_n \to \mathcal{B}(\mathcal{H}') \otimes \mathcal{M}_n \) is positive for all \( n \), where \( \mathcal{M}_n \) is the set of \( n \times n \) complex matrices.

1 The Quantum Formalism

In this section we will describe the mathematical formalism of quantum mechanics from an information theoretic point of view. For that, we will enunciate the postulates of quantum mechanics giving some immediate consequences of them and introducing also the key concepts of uncertainty, quantum channels and entanglement. For a full review see, for example, [1, 3].

1.1 Systems and States

Postulate 1: Associated to every physical system there is a complex Hilbert space \( \mathcal{H} \), that is known as the state space of the system. The system is described by its state, which is a density operator of the state space.

We denote physical system by capital letters \( A, B \) and \( C \) or numbers if there is an implicit order. Their Hilbert space is denoted by \( \mathcal{H}_A, \mathcal{H}_B \) and \( \mathcal{H}_C \) respectively and their density operator is denoted by greek letters \( \rho_A, \sigma_B \).

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1 This representation is not unique as it was for pure states (up to normalization).
and $\tau_C$ where the subindices will be removed if the system is clear from the context. The dimension of the physical system is given by the dimension of the Hilbert space associated to it.

The easiest quantum system one could think of is a two dimensional system, whose state space is $\mathbb{C}^2$. Let $\{|0\rangle, |1\rangle\}$ be an orthonormal basis of $\mathbb{C}^2$, an arbitrary pure state can be written as $|\psi\rangle = a|0\rangle + b|1\rangle$ with $|a|^2 + |b|^2 = 1$. The physical system can be in the state $|0\rangle$ and in the state $|1\rangle$, but also in a superposition of both $|\psi\rangle$. Despite its simplicity, this system is of extremely importance as it is the unit of information in quantum systems. Such a system is called quantum bit or qubit in analogy to the fundamental unit of classical information called bit. A $d$-dimensional quantum system or qudit will be represented in $\mathbb{C}^d$ and its pure states will be described in terms of an orthonormal basis of $d$ elements $|1\rangle, |2\rangle, \ldots, |d\rangle$.

Postulate 2: The state space of a composite physical system $\mathcal{H}$ is the tensor product of the state spaces $\{\mathcal{H}_i\}$ of the component physical systems. Moreover, if we have systems labeled from 1 to $n$ and system $i$ is prepared in the state $\rho_i$, then the state of the total system is $\rho_1 \otimes \cdots \otimes \rho_n$.

We write $\rho_{AB}$ for the density operator of a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$ to stress that is a composite system of subsystems $A$ and $B$. The state of system $A$ when considered alone is given by its reduced density operator $\rho_A := \text{tr}_B \rho_{AB}$, where the partial trace operator $\text{tr}_B : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{B}(\mathcal{H}_A)$ is defined as the unique linear operator such that
\[ \text{tr}_B (R \otimes S) = (1 \otimes \text{tr})(R \otimes S) = R \text{ tr} (S), \quad \forall R \in \mathcal{B}(\mathcal{H}_A), \forall S \in \mathcal{B}(\mathcal{H}_B). \]

One can also define the reduced density operator of system $B$, $\rho_B$, interchanging the roles of systems $A$ and $B$. Moreover, if we have a composite system of several subsystems the reduced state of a set of them $X$ is given by considering the partial trace over the others. That is, $\rho_X = \text{tr}_{A_{\bar{X}}} \rho$.

We say that a pure state $|\varphi\rangle_{1,\ldots,n}$ of a composite system $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is in a product state if it can be written as a tensor product of elementary tensors in each of the systems, that is, $|\varphi\rangle_{1,\ldots,n} = |\varphi_1\rangle \cdots |\varphi_n\rangle$, where $|\varphi_i\rangle \in \mathcal{H}_i$ for all $i$. This concept generalizes to mixed states as separable states. We say that a mixed state is separable if it can be written as a convex combination of tensor product of density operators. That is, a density operator $\rho_{1,\ldots,n}$ acting on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is separable if there exist $p_k \geq 0$ with $\sum_k p_k = 1$ and density operators $\{\rho_i^k\}_{i,k}$ acting on $\mathcal{H}_i$ respectively such that
\[ \rho_{1,\ldots,n} = \sum_k p_k \rho_1^k \otimes \cdots \otimes \rho_n^k. \]
If a density operator is not separable we say that it is entangled. Examples of entangled pure states of two qubits are the so-called Bell states or Einstein-Podolski-Rosen (EPR) pairs

\[
\frac{|00\rangle + |11\rangle}{\sqrt{2}}, \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \frac{|00\rangle - |11\rangle}{\sqrt{2}} \text{ and } \frac{|01\rangle - |10\rangle}{\sqrt{2}}.
\] (1)

We will use the following conventions for qubits. The computational basis \(\{|0\>, |1\rangle\} \) is given by \(|0\rangle = (1, 0)^T\) and \(|1\rangle = (0, 1)^T\) and the Hadamard basis by \(\{H|0\rangle, H|1\rangle\}\), where \(H\) denotes the 2-dimensional Hadamard matrix

\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

We also call the computational basis the plus basis and associate it with the ‘+’-symbol, and we call the Hadamard basis the times basis and associate it with the ‘×’-symbol. For bit vectors \(x = (x_1, \ldots, x_n) \in \{0, 1\}^n\) and \(v = (v_1, \ldots, v_n) \in \{+, \times\}^n\) we then write \(|x\rangle_v = |x_1\rangle_{v_1} \otimes \cdots \otimes |x_n\rangle_{v_n}\), where \(|x_i\rangle_+ := |x_i\rangle\) and \(|x_i\rangle_\times := H|x_i\rangle\).

A convenient basis for operators on \(\mathbb{C}^2\) is given by the set of Hermitian matrices formed by the identity matrix and the 3 Pauli matrices.

\[
\sigma_0 = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\] (2)

The following proposition gives a way to write systems of two subsystems.

**Proposition 1.1 (Schmidt decomposition).** Let \(|\psi\rangle_{AB} \in \mathbb{C}^d \otimes \mathbb{C}^n\) with \(n \geq d\). There exist orthonormal bases \(\{|u_1\rangle, \ldots, |u_d\rangle\} \subset \mathbb{C}^d\) and \(\{|v_1\rangle, \ldots, |v_n\rangle\} \subset \mathbb{C}^n\) such that \(|\psi\rangle = \sum_{i=1}^k \lambda_i |u_i\rangle \otimes |v_i\rangle\) where \(\lambda_i \geq 0\) for all \(i\), \(\sum_{i=1}^{k} \lambda_i^2 = 1\) and \(k \leq d\). Such a way of writing the state is called Schmidt decomposition, \(\lambda_1, \ldots, \lambda_k\) are the Schmidt coefficients and the number of summands in such a decomposition is called the Schmidt rank of \(|\psi\rangle\).

This proposition is a straightforward consequence of the singular value decomposition (SVD) of a matrix and thus the Schmidt rank and coefficients are unique and the freedom in the basis is given by the freedom in the SVD. It is clear that the reduced density matrices of the state \(|\psi\rangle_{AB}\) will be \(\rho_A = \sum_{i=1}^n \lambda_i^2 |u_i\rangle \langle u_i|\) and \(\rho_B = \sum_{i=1}^n \lambda_i^2 |v_i\rangle \langle v_i|\).

Given a density matrix \(\rho_A \in \mathcal{B}(\mathbb{C}^d)\) of a system A, it can be diagonalized and written as \(\rho_A = \sum_{i=1}^d \lambda_i |i\rangle \langle i|\) for some orthonormal basis \(\{|i\rangle\}\). Consider another system B of the same dimension, then \(\rho_A = \text{tr}_B |\psi\rangle_{AB}\) where \(|\psi\rangle_{AB} = \sum_{i=1}^d \sqrt{\lambda_i} |i\rangle_A |i\rangle_B\). We say that \(|\psi\rangle_{AB}\) is a purification of the state \(\rho_A\).
1. THE QUANTUM FORMALISM.

1.2 Quantum Transformations: Evolution and Measurement

Postulate 3: The time evolution of a closed quantum system is described by the Schrödinger equation,

\[ i \frac{d|\psi\rangle}{dt} = H|\psi\rangle \]

where \( H \) is a hermitian operator known as the Hamiltonian of the system\(^2\) This postulate extends to density operators by linearity.

The Hamiltonian has a spectral decomposition \( H = \sum_i E_i |\psi_i\rangle \langle \psi_i| \) with eigenvalues \( E_i \) and associated eigenstates \( |\psi_i\rangle \). States \( |\psi_i\rangle \) are called stationary states with energy \( E_i \) and the eigenstates of lowest energy are known as the ground states of the system. The solution to the Schrödinger equation for a certain time is given by

\[ |\psi(t_2)\rangle = e^{-iH(t_2-t_1)}|\psi(t_1)\rangle, \]

and thus stationary states are invariant in time up to a phase. Moreover, the states \( \rho(t_1) \) and \( \rho(t_2) \) of the system in times \( t_1 \) and \( t_2 \) respectively, are related by

\[ \rho(t_2) = U(t_1, t_2) \rho(t_1) U^\dagger(t_1, t_2), \]

where \( U(t_1, t_2) = e^{-iH(t_2-t_1)} \) is a unitary operator of the state space \( \mathcal{H} \), which only depends on times \( t_1 \) and \( t_2 \). Thus, whenever we want to describe the evolution between two fixed times we will just work with a unitary operator.

Postulate 3 describes the evolution of closed quantum systems. However, we also need to describe the change of a system when one tries to observe it to gain some information about it. In this case, the system is no longer closed as the apparatus or the observer himself are interacting in some way with the system. This process of measurement is described by the following postulate.

Postulate 4: The measurement of a system is described by a collection of measurement operators \( \{M_m\} \) that act in the state space of the system \( \mathcal{H} \). The index \( m \) refers to the possible outcomes of the measurement. If the state of a quantum system is \( \rho \) immediately before the measurement then the result of the measurement is \( m \) with probability \( p(m) = \text{tr} (M_m^\dagger M_m \rho) \). The state of the system after the measurement have outcome \( m \) is

\[ \rho_m = \frac{M_m \rho M_m^\dagger}{p(m)}. \]

\(^2\)We consider the Planck's constant inside \( \mathcal{H} \).
The measurement operators satisfy the completeness equation, $\sum_{m} M^\dagger_m M_m = 1$, which translates in probabilities of the results summing 1.

A measurement is a map that takes as input a state $\rho$ and returns the state $\rho_i$ with probability $p_i$, that is, it returns the ensemble of states $\{p_i, \rho_i\}$, where $\rho_i$ can be mixed or pure states. Note that, $\rho = \sum_i p_i \rho_i$ by the completeness equation. Thus, it has full meaning to consider the state $\rho$ as an statistical ensemble of the states $\rho_i$ with probability $p_i$. Mixed states have attached the idea of some ignorance about the system beyond that of the probability distribution. A discrete probability distribution $\{p_i\}_i$ can be represented as $\rho = \sum_i p_i |i\rangle\langle i|$ where $\{|i\rangle\}$ is an orthonormal basis of the Hilbert space. If we measure the state $\rho$ in that basis, that is, with measurement operators $\{|i\rangle\langle i|\}_i$, we will obtain the result $i$ with probability $p_i$. We say that the state $\rho$ models a classical system or simply that it is classical. In this way, one can see classical probability distributions inside quantum states.

We say that a measurement is a Von Neumann measurement if the measurement operators are orthogonal projections. Restrict to Von Neumann measurements is not formally a restriction as one can represent a general measurement as a Von Neumann measurement in a larger system via Neu- mark’s dilation theorem [2].

In certain cases in which one is not interested in the state after the measurement it will be convenient to use the so called POVM (positive operator-valued measurement) formalism in which the measurement is described by an observable. An observable $O$ is a linear functional acting on $D_1(\mathcal{H})$ given by a set of positive operators $E_m$, with $\sum_m E_m = 1$, such that $O = \sum_m m E_m$. In this case the probability of the result $m$ to occur is $p(m) = \text{tr}(E_m \rho)$ and the expected value of the measurement is given by the observable $\langle O \rangle = O(\rho) = \text{tr}(O \rho) = \sum_m mp_m$. 

Bibliography

