

TCM315 Fall 2022: Introduction to Open Quantum Systems

Lecture 4: The postulates of Quantum Mechanics

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INTRODUCTION

The function of postulates in a physical theory is to act as a bridge between physics and mathematics. They specify *correspondence rules* between the physical models and the mathematical tools. Once these rules are fixed, the analysis of the physical model turns into a well defined mathematical problem.

In the literature there exists several formulations of the postulates. Although they lead to the same mathematical theory, the emphasis in different formulations may reflect distinct attitudes towards *physical interpretation*. The *ontology* (i.e. the nature of being of the physical entities described by the mathematical theory) of different interpretations of quantum mechanics still remains a controversial topic, open for further investigations. A balanced presentation aimed at the *general reader* of the problems inherent to the interpretation of Quantum Mechanics, from its inception to the present may be found in [8]. A recommended reading for further deepening of the study is the now classic collection of papers by John Bell [4].

In order to avoid technical aspect of functional analysis we set the focus on Quantum Mechanical models with a finite number of states as in [11]. We, however, make some remarks to warn about the source of difficulties arising

when considering the infinite dimensional case [9]. A good mathematical reference for the general case is [10] and together with the evergreen classic [12].

THE POSTULATES

The postulates appear in different order and number in the literature. Here we mainly draw from [11] which is widely regarded as classic reference for quantum computation and information. The reason for referring to [11] is that it appears to us to have a neat “**for all practical purposes**” (F.A.P.P.) attitude towards the postulates. This means that the postulates are regarded as nothing more than set of rules to make computations in Quantum Mechanics. Concerning the interpretation we frankly state here that we regard the co-existence of two dynamical postulates unitary evolution and measurement postulate as the indication of an open problem in physics [2, 7]. We believe that advances in physics are intertwined with the eventual emergence of new experimental evidences whereas we are unconvinced by attempts to circumvent problems in physics by subtle philosophical arguments.

THE "KINEMATIC" POSTULATES

The kinematic postulates set the scene and define the characters playing a role in Quantum Mechanics.

The state space

Postulate (Hilbert Space).

The **state space** of an isolated physical system is mathematically described by a **Hilbert space** \mathcal{H} . For all practical purposes, the system is completely described by its state vector, which is a **unit ray** in the system's Hilbert space.

Hilbert space

Definition. A (complex) Hilbert space is a complete complex vector space \mathcal{H} with an inner product.

The adjective **complete** refers to the technical requirement that every sequence converging in **Cauchy sense** is also **converging**. This requirement is important in abstract formulations, but we does not play any explicit role in the explicit cases we will consider.

In the absence of further notice, we work with **finite dimensional** Hilbert spaces e.g.

$$\mathcal{H} \sim \mathbb{C}^d$$

The dimension d may-be however very large e.g. $O(10^9)$. Eventually, we will consider the limit d tending to infinity and related “continuum” limit. In these latter cases we will deal only with explicit examples without attempting to expounding systematically the theory.

For a vector in \mathcal{H} we will use the simple notation ψ . The inner product is a linear map $\mathcal{H} \times \mathcal{H} \mapsto \mathbb{C}$ between two elements ψ, ϕ of \mathcal{H}

$$\phi^\dagger \psi = \sum_{i=1}^d \bar{\phi}_i \psi_i \quad (1)$$

with the sum thus ranging over all vector components and $\bar{\phi}_i$ is the **complex conjugate** of ϕ_i . In other words \dagger means transposition \top and complex conjugation of a column vector.

Remark. An inner product notation often used in mathematics is

$$\langle \psi, \psi \rangle_{\mathbb{C}^d} = \psi^\dagger \psi$$

where the bracket subscript, if present specifies the space. Thus if the Hilbert space is that of the square integrable functions on the real line $\mathcal{H} = \mathbb{L}^2(\mathbb{R}^d)$ then

$$\langle \phi, \psi \rangle_{\mathbb{L}^2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} d^d x \phi^*(\mathbf{x}) \psi(\mathbf{x})$$

Note that Cauchy-Schwarz inequality insures that the so defined inner product is finite in $\mathbb{L}^2(\mathbb{R}^d)$. The subscript is omitted if no ambiguity arises concerning the Hilbert space in consideration.

* *

Any abstract inner product must enjoy the following properties which we straightforwardly verify for the explicit case (1)

1. positivity: for all ψ in \mathcal{H}

$$\psi^\dagger \psi = \|\psi\|^2 \geq 0$$

in particular

$$\|\psi\|^2 = 0 \quad \iff \quad \psi = 0$$

2. linearity : for all **c-numbers** i.e. $c_1, c_2 \in \mathbb{C}$ and elements of the Hilbert space ϕ and ψ_1, ψ_2

$$\phi^\dagger \left(\sum_{i=1}^2 c_i \psi_i \right) = \sum_{i=1}^2 c_i \phi^\dagger \psi_i$$

3. anti-linearity: for all **c-numbers** i.e. $c_1, c_2 \in \mathbb{C}$ and elements of the Hilbert space ϕ and ψ_1, ψ_2

$$\left(\sum_{i=1}^2 c_i \psi_i \right)^\dagger \phi = \sum_{i=1}^2 \bar{c}_i \psi_i^\dagger \phi$$

4. skew symmetry: for all ψ, ϕ in \mathcal{H}

$$(\phi^\dagger \psi)^\dagger = \psi^\dagger \phi$$

Rays and unit vectors

In the Hilbert state postulate we write that the complete description of the state of the system is encoded in a **unit ray**. This means that for any $\theta \in \mathbb{R}$ the state vector

$$\tilde{\psi} = e^{i\theta} \psi$$

contains the same physical information as ψ both being subject to the same constraint

$$\tilde{\psi}^\dagger \tilde{\psi} = \psi^\dagger \psi = 1 \quad (2)$$

The condition (2) restrict states to an hyper-sphere of unit radius of the Hilbert space.

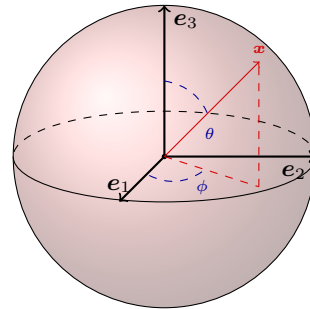
The states of a **two-level** quantum system take values on the **Bloch sphere**. If we denote by $\left\{ \mathbf{e}_i^{(2)} \right\}_{i=1}^2$ the canonical basis of \mathbb{C}^2

$$\mathbf{e}_1^{(2)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \& \quad \mathbf{e}_2^{(2)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

then we can write a generic state on the Bloch sphere as

$$\psi = \cos \frac{\theta}{2} \mathbf{e}_1^{(2)} + e^{i\phi} \sin \frac{\theta}{2} \mathbf{e}_2^{(2)}$$

$$0 \leq \theta < \pi \quad \& \quad 0 \leq \phi < 2\pi$$



Bloch sphere represented as the 2-sphere

Remark. Note that

$$\theta \in [0, \pi] \implies \cos \frac{\theta}{2} \geq 0 \ \& \ \sin \frac{\theta}{2} \geq 0$$

Hence ϕ determines the relative sign between the coefficients.

* *

We can also re-interpret the variables θ, ϕ as spherical coordinates on the 2-sphere

$$S^2 = \left\{ \mathbf{x} \in \mathbb{R}^3 \mid \mathbf{x}^\top \mathbf{x} \equiv \|\mathbf{x}\|^2 = 1 \right\}$$

so that if $\left\{ \mathbf{e}_i^{(3)} \right\}_{i=1}^3$ denotes the canonical basis of \mathbb{R}^3 we write

$$\mathbf{x} = \sin \theta \cos \phi \mathbf{e}_1^{(3)} + \sin \theta \sin \phi \mathbf{e}_2^{(3)} + \cos \theta \mathbf{e}_3^{(3)}$$

Dynamical variables and operators

The second postulate pertains the mathematical characterization of dynamical variables.

Postulate (Dynamical variables).

To each **dynamical variable** \mathcal{A} of a quantum system defined on \mathcal{H} there is a **self-adjoint** operator \mathbb{A} .

- The eigenvalues of \mathbb{A} specify the values of the dynamical variable, whose admissible values thus correspond to the spectrum of

$$\text{Sp } \mathbb{A} = \{a_1, \dots\}$$

- The eigenvectors of \mathbb{A} specify the probability that the dynamical variable takes one of its admissible values for a system specified by a state vector ψ . In particular, if \mathbb{A} admits the spectral decomposition

$$\mathbb{A} = \sum_{i \mid a_i \in \text{Sp } \mathbb{A}} a_i \mathbb{P}_{a_i}$$

where the sum ranges over the distinct eigenvalues and \mathbb{P}_{a_i} is the projector onto the vector subspace associated to the eigenvalue a_i , then

$$P(\mathcal{A} = a_i \mid \psi) = \|\mathbb{P}_{a_i} \psi\|^2 \tag{3}$$

In other words, the spectral projection onto a state determines the probability that the dynamical variables is equal to the eigenvalue **conditionally** to the fact that the system is in the state ψ .

It is very important to pay attention to the fact that the probability is a **conditional probability** with respect to the state: it is not an intrinsic property of the dynamical variable.

Self-adjoint operators play a special role because of the **spectral theorem** (see appendix) which guarantees that

- all eigenvalues are real,
- left and right eigenvectors coincide and form a **complete orthonormal basis** of the vector space.

In particular, the spectral theorem insures that the sum of the probability of all the admissible events adds up to one. Namely if \mathbb{A} has $N \leq d = \dim \mathcal{H}$ distinct eigenvalues, we readily obtain the chain of identities

$$1 = \psi^\dagger \psi = \psi^\dagger \left(\sum_{i=1}^N \mathbb{P}_{a_i} \right) \psi = \sum_{i=1}^N \psi^\dagger \mathbb{P}_{a_i} \psi = \sum_{i=1}^N (\mathbb{P}_{a_i} \psi)^\dagger \mathbb{P}_{a_i} \psi = \sum_{i=1}^N \|\mathbb{P}_{a_i} \psi\|^2 = \sum_{i=1}^N P(\mathcal{A} = a_i \mid \psi)$$

by recalling the idempotency

$$\mathbb{P}_{a_i}^2 = \mathbb{P}_{a_i}$$

and completeness

$$\sum_{i=1}^N \mathbb{P}_{a_i} = \mathbb{1}_d$$

self-adjointness

$$\mathbb{P}_{a_i}^\dagger = \mathbb{P}_{a_i}$$

properties of the spectral projectors. These properties are most clearly illustrated in the case when the spectrum of \mathbb{A} is **non-degenerate**. In such a case

$$\mathbb{A} = \sum_{i=1}^{\dim \mathcal{H}} a_i \mathbf{v}_i \mathbf{v}_i^\dagger$$

Remark. and Infinite dimensional formulation of Mechanics e.g. to $\mathbb{L}^{(2)}(\mathbb{R})$ must take into account several difficulties which can be addressed by resorting to functional analysis [10]. We list some of them [9].

- An operator in an infinite dimensional Hilbert space must always be thought as the pair $(A, \text{dom}(A))$ where A specifies the action on the Hilbert space vector

$$\phi = A \psi \quad (4)$$

and $\text{dom}(A) \subseteq \mathcal{H}$ the subset of the Hilbert space on which A is defined.

- Hermitian (in the mathematics literature often referred as “symmetric”) operators i.e. operators for which

$$A \psi = A^\dagger \psi \quad \forall \psi \in \text{dom}(A) \cap \text{dom}(A^\dagger)$$

are self-adjoint **only if** $\text{dom}(A) = \text{dom}(A^\dagger)$ also holds. In the finite dimensional case Hermitian and self-adjoint operators are equivalent concepts. In the infinite dimensional case, they are **not**.

- $\phi = A \psi$ may not belong to \mathcal{H} .
- A self-adjoint unbounded A operator **cannot** be defined on the full Hilbert space (this is a consequence of Hellinger–Toeplitz theorem see e.g. § 3.2 of [10] or [9]).

Infinite dimensional Hilbert space will occur in this course only in the form of explicit examples. This fact will allow us to evince and solve the difficulties associated to the infinite dimensionality of the space.

* *

Operator algebras

Besides self-adjoint operators associated to dynamical variables it is convenient to introduce the space $\mathcal{M}_d(\mathbb{C})$ of complex $d \times d$ matrices. We regard these matrices as **linear operators** on the Hilbert space $\mathcal{H} = \mathbb{C}^d$. We then notice that $\mathcal{M}_d(\mathbb{C})$ is itself an Hilbert space once we endow it with the **Hilbert-Schmidt inner product**

$$\langle \mathbb{A}, \mathbb{B} \rangle_{\mathcal{M}_d} \equiv \text{Tr } \mathbb{A}^\dagger \mathbb{B} \equiv \sum_{l,k=1}^d a_{kl}^* b_{kl}$$

The advantage of thinking of $\mathcal{M}_d(\mathbb{C})$ as an Hilbert space is that then it is natural to think as matrix elements as the coefficients of \mathbb{A} in a certain basis. For example, we can introduce the **canonical basis** as

$$\mathbb{E}_{ij}^{(d)} = \mathbf{e}_i^{(d)} \mathbf{e}_j^{(d)\dagger}$$

where $\{e_i^{(d)}\}_{i=1}^d$ is the canonical basis of \mathcal{H} . The Hilbert-Schmidt inner product then yields the orthonormality relations

$$\text{Tr } \mathbb{E}_{ij}^{(d)\dagger} \mathbb{E}_{lk}^{(d)} = \text{Tr} \left(e_j^{(d)} e_i^{(d)\dagger} e_l^{(d)} e_k^{(d)\dagger} \right) = e_k^{(d)\dagger} e_j^{(d)} e_i^{(d)\dagger} e_l^{(d)} = \delta_{jk} \delta_{il}$$

whence it is straightforward to verify

$$\mathbb{A} = \sum_{ij=1}^d a_{ij} \mathbb{E}_{ij}^{(d)}$$

An approach alternative to the Hilbert space representation, is to set the focus on the collection $\mathcal{B}(\mathcal{H})$ of the **bounded linear operators** acting on \mathcal{H} . In the finite dimensional case, this makes no difference because any operator is bounded. In the infinite dimensional case thinking in terms of $\mathcal{B}(\mathcal{H})$ turns out to be more fruitful. Namely it is possible to construe $\mathcal{B}(\mathcal{H})$ as a **normed space** rather than a space with inner product. The adapted choice of the norm is the **trace norm**

$$\|\mathbb{A}\|_1 = \text{Tr} \sqrt{\mathbb{A}^\dagger \mathbb{A}}$$

In mathematics a normed complete vector space is called a **Banach space**. The elements of $\mathcal{B}(\mathcal{H})$ then form an **algebra** closed with respect to

- multiplication by a c-number: if $\mathbb{A} \in \mathcal{B}(\mathcal{H})$ then $c\mathbb{A} \in \mathcal{B}(\mathcal{H})$ for any $c \in \mathbb{C}$.
- addition: if $\mathbb{A}_1, \mathbb{A}_2 \in \mathcal{B}(\mathcal{H})$ then $\mathbb{A}_1 + \mathbb{A}_2 \in \mathcal{B}(\mathcal{H})$.
- multiplication: if $\mathbb{A}_1, \mathbb{A}_2 \in \mathcal{B}(\mathcal{H})$ then $\mathbb{A}_1 \mathbb{A}_2 \in \mathcal{B}(\mathcal{H})$.

The algebra is non-commutative because in general

$$[\mathbb{A}_1, \mathbb{A}_2] = \mathbb{A}_1 \mathbb{A}_2 - \mathbb{A}_2 \mathbb{A}_1 \neq 0$$

Finally, we emphasize that the \dagger operation (transposition and complex conjugation) satisfies on $\mathcal{B}(\mathcal{H})$ the following properties

1. $(\mathbb{A}_1 + \mathbb{A}_2)^\dagger = \mathbb{A}_1^\dagger + \mathbb{A}_2^\dagger$
2. $(\mathbb{A}_1 \mathbb{A}_2)^\dagger = \mathbb{A}_2^\dagger \mathbb{A}_1^\dagger$
3. $\mathbb{1}_d^\dagger = \mathbb{1}_d$
4. $(\mathbb{A}^\dagger)^\dagger = \mathbb{A}$

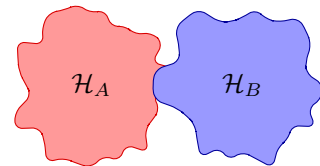
These four properties specify the requirements that an abstract $*$ operation must satisfy. Thus the algebra $\mathcal{B}(\mathcal{H})$ of bounded (equivalently continuous) linear operators defined on a complex Hilbert space \mathcal{H} provides a prototypical example of a C^* algebra. C^* algebras provide an abstract mathematical setting to describe classical and quantum mechanics on the same footing. A brief overview of this concepts is contained in chapter 5 of [1] whereas [5, 6] are the standard references for the full mathematical theory.

Composite systems

Composite systems are systems consisting of different parts which we know how to treat when are separated. The composite system postulate tells us how to combine the degrees of freedom of the different parts.

Postulate (Tensor product).

The state space is the **tensor product** of the state spaces of the component physical systems



$$\mathcal{H}_{A+B} = \mathcal{H}_A \otimes \mathcal{H}_B$$

$$\dim \mathcal{H}_{A+B} = \dim \mathcal{H}_A \times \dim \mathcal{H}_B$$

To illustrate the meaning of the tensor product operation we denote by $\{e_i^{(d_A)}\}_{i=1}^{d_A}$ the canonical basis of the Hilbert space \mathcal{H}_A with dimension d_A . Similarly, we suppose that $\{e_i^{(d_B)}\}_{i=1}^{d_B}$ is the canonical basis of the Hilbert space \mathcal{H}_B . We write generic elements of the two spaces as

$$\mathbf{a} = \sum_{i=1}^{d_A} a_i e_i^{(d_A)}$$

and

$$\mathbf{b} = \sum_{i=1}^{d_B} b_i e_i^{(d_B)}$$

where the collections of c-numbers $\{c_i^{(A)}\}_{i=1}^{d_A}$ and $\{c_i^{(B)}\}_{i=1}^{d_B}$ are respectively the components of \mathbf{a} and \mathbf{b} in the canonical bases. The tensor product

$$\mathbf{a} \otimes \mathbf{b} = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} a_i b_j e_i^{(d_A)} \otimes e_j^{(d_B)}$$

then specifies a vector in the \mathcal{H}_{A+B} Hilbert space with dimension

$$d_{A+B} = d_A \times d_B$$

We adopt the convention to relate the canonical bases of these spaces according to the relation

$$e_{(i-1)d_B+j}^{(d_{A+B})} \sim e_i^{(d_A)} \otimes e_j^{(d_B)} \quad (5)$$

Using the column representation this means that in the $d_A = d_B = 2$ case we have

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \otimes \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} a_1 \otimes \mathbf{b} \\ a_2 \otimes \mathbf{b} \end{bmatrix} = \begin{bmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{bmatrix}$$

We can immediately apply (5) to define the tensor product of matrices. Namely, if we represent the canonical basis of \mathcal{M}_{d_A} as

$$\mathbb{E}_{ij}^{(d_A)} = e_i^{(d_A)} e_j^{(d_A)\dagger}$$

then

$$\mathbb{E}_{ij}^{(d_A)} \otimes \mathbb{E}_{lk}^{(d_B)} = e_i^{(d_A)} e_j^{(d_A)\dagger} \otimes e_l^{(d_B)} e_k^{(d_B)\dagger} = \left(e_i^{(d_A)} \otimes e_l^{(d_B)} \right) \left(e_j^{(d_A)\dagger} \otimes e_k^{(d_B)\dagger} \right)$$

implies that in accordance with the adoption of (5) we set

$$\mathbb{E}_{(i-1)d_B+l(j-1)d_B+k}^{(d_A \times d_B)} = e_{(i-1)d_B+l}^{(d_A \times d_B)} e_{(j-1)d_B+k}^{(d_A \times d_B)\dagger}$$

In the $d_A = d_B = 2$ case, this concretely means that for

$$\mathbb{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \quad \& \quad \mathbb{B} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

then

$$\mathbb{A} \otimes \mathbb{B} = \begin{bmatrix} a_{11} \otimes \mathbb{B} & a_{12} \otimes \mathbb{B} \\ a_{21} \otimes \mathbb{B} & a_{22} \otimes \mathbb{B} \end{bmatrix} = \begin{bmatrix} a_{11} b_{11} & a_{11} b_{12} & a_{12} b_{11} & a_{12} b_{12} \\ a_{11} b_{21} & a_{11} b_{22} & a_{12} b_{21} & a_{12} b_{22} \\ a_{21} b_{11} & a_{21} b_{12} & a_{22} b_{11} & a_{22} b_{12} \\ a_{21} b_{21} & a_{21} b_{22} & a_{22} b_{21} & a_{22} b_{22} \end{bmatrix}$$

THE "DYNAMICAL" POSTULATES

There is wide consensus that conceptual difficulties in the interpretation of Quantum Mechanics originate in the apparent coexistence of two dynamical evolution principles without non-contextual a-priori definition of their respective domain of applicability [2, 3].

Unitary evolution

Postulate. *The evolution of a closed quantum system is described by a **unitary transformation**. That is, the state vector ψ_{t_1} of the system at time t_1 is related to the state ψ_{t_2} of the system at time t_2 by a unitary operator \mathbb{U} which depends only on the times t_1 and t_2*

In formulas the postulate tells us that

$$\psi_{t_2} = \mathbb{U}_{t_2 t_1} \psi_{t_1}$$

Unitary evolution **preserves** probability

$$\psi_{t_2}^\dagger \psi_{t_2} = \psi_{t_1}^\dagger \psi_{t_1}$$

The relation must hold for any $t_1, t_2 \in \mathbb{I}$ where \mathbb{I} is the time interval during which the evolution occurs. As a consequence, the time evolution operator of a quantum system must enjoy the two parameter group property

1. composition property $\mathbb{U}_{t_3 t_1} = \mathbb{U}_{t_3 t_2} \mathbb{U}_{t_2 t_1}$
2. existence of the inverse $\mathbb{U}_{t_2 t_1}^{-1} = \mathbb{U}_{t_2 t_1}^\dagger = \mathbb{U}_{t_1 t_2}$
3. existence of the identity $\mathbb{U}_{t t} = \mathbb{1}$ for all t .

The Hamiltonian operator is the generator of the unitary dynamics

We denote by

$$\dot{\mathbb{U}}_{t t_0} = \frac{d}{dt} \mathbb{U}_{t t_0}$$

Proposition. *The operator product $\dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger$ is independent of t_0 . We call the **generator** of the unitary evolution*

$$\mathbb{H}_t := i \dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger$$

*the **Hamiltonian operator**. By definition the Hamiltonian operator is self-adjoint:*

$$\mathbb{H}_t = \mathbb{H}_t^\dagger$$

Proof. To check the first claim we write

$$\dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger = \lim_{s \downarrow 0} \frac{\mathbb{U}_{t+s t_0} - \mathbb{U}_{t t_0}}{s} \mathbb{U}_{t t_0}^\dagger = \lim_{s \downarrow 0} \frac{\mathbb{U}_{t+s t_0} \mathbb{U}_{t t_0}^\dagger - \mathbb{1}}{s} = \lim_{s \downarrow 0} \frac{\mathbb{U}_{t+s t} - \mathbb{1}}{s}$$

The rightmost term is readily independent of t_0 . We then avail us of the definition of unitary matrix

$$0 = \frac{d}{dt} (\mathbb{U}_{t t_0} \mathbb{U}_{t t_0}^\dagger) = \dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger + \mathbb{U}_{t t_0} \dot{\mathbb{U}}_{t t_0}^\dagger$$

shows that

$$\dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger = -\mathbb{U}_{t t_0} \dot{\mathbb{U}}_{t t_0}^\dagger$$

Hence, the chain of identities

$$\mathbb{H}_t^\dagger = \left(i \dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger \right)^\dagger = -i \mathbb{U}_{t t_0} \dot{\mathbb{U}}_{t t_0}^\dagger = -i \left(-\dot{\mathbb{U}}_{t t_0} \mathbb{U}_{t t_0}^\dagger \right) = \mathbb{H}_t$$

□

Schrödinger's equation

Once we have identified the Hamiltonian as the generator of the dynamics, we are ready to derive the infinitesimal version of the postulate: the **Schrödinger equation**. To this goal we observe that the chain of identities

$$\frac{d}{dt}\psi_t = \frac{d}{dt}\mathbb{U}_{t t_0}\psi_{t_0} = -i(i\dot{\mathbb{U}}_{t t_0}\mathbb{U}_{t t_0}^\dagger)\mathbb{U}_{t t_0}\psi_{t_0} = -i\mathbb{H}_t\psi_t$$

yields

$$i\frac{d}{dt}\psi_t = \mathbb{H}_t\psi_t$$

In the infinite dimensional case this result is the contents of the Stone – von Neumann theorem [10].

In case \mathbb{H} is time independent, the solution of the Schrödinger equation with initial data at $t_0 = 0$ reads

$$\psi_t = e^{-i\mathbb{H}t}\psi_0$$

In the time-non autonomous case, the solution of the Schrödinger equation takes the form of a **time ordered exponential**

$$\psi_t = \overleftarrow{\mathcal{T}} \exp\left(-i\int_0^t ds \mathbb{H}_s\right)\psi_0 = \psi_0 + \sum_{i=1}^{\infty}(-i)^i \prod_{j=1}^i \int_0^t ds_j \overleftarrow{\mathcal{T}}\left(\prod_{k=1}^i \mathbb{H}_{s_k}\right)$$

where

$$\overleftarrow{\mathcal{T}}\left(\prod_{k=1}^i \mathbb{H}_{t_k}\right) = \begin{cases} \mathbb{H}_{t_i}\mathbb{H}_{t_{i-1}}\dots\mathbb{H}_{t_1} & \text{if } t_i \geq t_{i-1} \geq \dots \geq t_1 \\ 0 & \text{otherwise} \end{cases}$$

From the physics slant, the Hamilton operator \mathbb{H}_t is specified by modeling.

In summary, the family of unitary transformations $\mathbb{U}_{t t_0}$ are the fundamental solution of the differential problem

$$i\frac{d}{dt}\mathbb{U}_{t t_0} = \mathbb{H}_t\mathbb{U}_{t t_0} \quad \& \quad \mathbb{U}_{t_0 t_0} = \mathbb{1}_d \quad (6)$$

Time reversal

Upon applying the adjoint operation to (6) we get into

$$-i\frac{d}{dt}\mathbb{U}_{t_0 t} = \mathbb{U}_{t_0 t}\mathbb{H}_t \quad \& \quad \mathbb{U}_{t_0 t_0} = \mathbb{1}$$

whence the interpretation of the adjoint operation as time-reversal.

The generalized measurement postulate

Postulate (Non unitary collapse). *We consider an experiment having \mathcal{M} distinct possible random outcomes. We suppose that*

- *to the i -th outcome is associated an operator \mathbb{M}_i on \mathcal{H} so that*

$$\sum_{k=1}^{\mathcal{M}} \mathbb{M}_k^\dagger \mathbb{M}_k = \mathbb{1}_d \quad d = \dim \mathcal{H} \quad (7)$$

Then in consequence of the measurement the following two statements hold true.

- If the i -th outcome is observed, the state instantaneously collapses to a new value

$$\psi_t \rightarrow \psi'_{t+dt} = \frac{\mathbb{M}_i \psi_t}{\|\mathbb{M}_i \psi_t\|}$$

- The probability to observe the i -th outcome is

$$\Pr\left(i\text{-th outcome} \middle| \psi_t\right) = \|\mathbb{M}_i \psi_t\|^2 \quad (8)$$

We notice that the products

$$\mathbb{E}_i = \mathbb{M}_i^\dagger \mathbb{M}_i \quad i = 1, \dots, \mathcal{M}$$

are usually called **effects**. The generalized measurement postulate thus requires the effect completeness relation

$$\mathbb{1}_d = \sum_{k=1}^{\mathcal{M}} \mathbb{E}_k$$

where we emphasize that \mathcal{M} **does not need to satisfy** any relation with $d = \dim \mathcal{H}$. In other words, \mathcal{M} can be smaller, equal or larger than d .

The simplest case is **projective** or **von-Neumann** measurement. This is the case of the ideal measurement of a dynamical variable \mathcal{A} mathematically described by a self-adjoint operator \mathbb{A} with non-degenerate spectrum

$$\text{Sp } \mathbb{A} = \{a_1, \dots, a_d\} \quad d = \dim \mathcal{H}$$

and

$$\mathbb{A} \mathbf{v}_i = a_i \mathbf{v}_i$$

Then we identify

$$\mathbb{M}_i = \mathbf{v}_i \mathbf{v}_i^\dagger$$

and the completeness relation (7) immediately follows from property of the eigenvectors of constituting a complete orthonormal system of \mathcal{H} in accordance with the spectral theorem. In this case (8) is simply a repetition of (3). In fact, we could have omitted (8) from the statement of the postulate as a redundancy because it is possible to prove that generalized measurement can be expressed in terms of a projective measurement.

The advantage of the generalized measurement described in the postulate is that it takes into account realistic situations when the outcome of a measurement does not give a definite result. To clarify the situation we observe that

Proposition. *Non orthogonal quantum states cannot be reliably distinguished.*

Proof. The proof goes by contradiction. Suppose we can devise a measurement able to distinguish between the two **unit non-orthonormal** states ψ_1, ψ_2 . Then it must be possible to construct two effects

$$\mathbb{E}_1 = \mathbb{M}_1^\dagger \mathbb{M}_1 \quad \& \quad \mathbb{E}_2 = \mathbb{M}_2^\dagger \mathbb{M}_2$$

such that

$$\mathbb{E}_1 + \mathbb{E}_2 = \mathbb{1}$$

and

$$\|\mathbb{M}_1 \psi_1\|^2 = \psi_1^\dagger \mathbb{E}_1 \psi_1 = 1 \quad \& \quad \|\mathbb{M}_2 \psi_2\|^2 = \psi_2^\dagger \mathbb{E}_2 \psi_2 = 1$$

If these hypotheses hold, then we must have

$$0 = \psi_1^\dagger \mathbb{E}_2 \psi_1 = \|\mathbb{M}_2 \psi_1\|^2 \quad \iff \quad \mathbb{M}_2 \psi_1 = 0$$

and therefore

$$\mathbb{E}_2 \boldsymbol{\psi}_1 = 0$$

By hypothesis $\boldsymbol{\psi}_1, \boldsymbol{\psi}_2$ are not orthonormal. Hence we can invoke Gram–Schmidt’s orthonormalization to write

$$\boldsymbol{\psi}_2 = c_1 \boldsymbol{\psi}_1 + c_2 \mathbf{u} \quad (9)$$

where \mathbf{u} is a **unit vector** such that

$$\boldsymbol{\psi}_1^\dagger \mathbf{u} = 0$$

and for some $c_1, c_2 \in \mathbb{C}$. Note that (9) implies

$$1 = |c_1|^2 + |c_2|^2$$

meaning that any $|c_1| > 0$ imposes $|c_2| < 1$. Furthermore, effects’ completeness relation implies

$$1 = \mathbf{u}^\dagger \mathbb{E}_1 \mathbf{u} + \mathbf{u}^\dagger \mathbb{E}_2 \mathbf{u} \quad \implies \quad 1 \geq \mathbf{u}^\dagger \mathbb{E}_2 \mathbf{u}$$

In consequence of these observations the chain of relations

$$\begin{aligned} 1 &= \boldsymbol{\psi}_2^\dagger \mathbb{E}_2 \boldsymbol{\psi}_2 = (c_1 \boldsymbol{\psi}_1 + c_2 \mathbf{u})^\dagger \mathbb{E}_2 (c_1 \boldsymbol{\psi}_1 + c_2 \mathbf{u}) \\ &= c_2 (c_1 \boldsymbol{\psi}_1 + c_2 \mathbf{u})^\dagger \mathbb{E}_2 \mathbf{u} = c_2 (\mathbb{E}_2 (c_1 \boldsymbol{\psi}_1 + c_2 \mathbf{u}))^\dagger \mathbf{u} = |c_2|^2 (\mathbb{E}_2 \mathbf{u})^\dagger \mathbf{u} \equiv |c_2|^2 \mathbf{u}^\dagger \mathbb{E}_2 \mathbf{u} \leq |c_2|^2 \end{aligned}$$

holds true. We thus arrive at a contradiction for any $c_1 \neq 0$. □

The lesson to be drawn is that there are situations when sometimes experimental outcomes do not permit to identify the state of the system.

An example of generalized measurement

Let us consider for example a quantum two level system. We identify the state vectors of the two levels with the elements of the canonical basis of \mathbb{C}^2 . We suppose that the effects of a generalized measurement are

$$\begin{aligned} \mathbb{E}_1 &= \frac{\sqrt{2}}{1 + \sqrt{2}} \mathbf{e}_2 \mathbf{e}_2^\dagger \\ \mathbb{E}_2 &= \frac{\sqrt{2}}{1 + \sqrt{2}} \frac{(\mathbf{e}_1 - \mathbf{e}_2)(\mathbf{e}_1 - \mathbf{e}_2)^\dagger}{2} \\ \mathbb{E}_3 &= \mathbb{1}_2 - \mathbb{E}_1 - \mathbb{E}_2 \end{aligned}$$

We see that the number of effects exceeds the number of dimensions of the Hilbert space. We also notice that

$$\Pr(\text{outcome } 1 \mid \mathbf{e}_1) = \mathbf{e}_1^\dagger \mathbb{E}_1 \mathbf{e}_1 = 0$$

This means that if the result of the measurement produces the outcome 1 then one can safely exclude that the state of the system be

$$\boldsymbol{\psi} = \mathbf{e}_1$$

Similarly, in the presence of outcome 2 we can rule out

$$\boldsymbol{\psi} = \frac{\mathbf{e}_1 + \mathbf{e}_2}{\sqrt{2}}$$

APPENDICES

Spectral theorem in the finite dimensional case

We review the spectral theorem in the finite dimensional case.

Normal operators

Definition. Normal operator. A normal operator on a complex Hilbert space \mathcal{H} is a continuous linear operator

$$[\mathbb{A}, \mathbb{A}^\dagger] \equiv \mathbb{A} \mathbb{A}^\dagger - \mathbb{A}^\dagger \mathbb{A} = 0$$

We notice that if \mathbb{A} is normal then $\tilde{\mathbb{A}} = \mathbb{A} - c \mathbb{1}$ for $c \in \mathbb{C}$ is also normal. Then we have:

Proposition. Eigenvectors of a normal operator. Let $k = 1, \dots, d$ labels eigenvalues and eigenvectors of \mathbb{A}

$$\mathbb{A} \mathbf{v}_k = \alpha_k \mathbf{v}_k \quad \Leftrightarrow \quad \mathbb{A}^\dagger \mathbf{v}_k = \alpha_k^* \mathbf{v}_k$$

Proof.

For any normal operator and any $\mathbf{v} \in \mathcal{H}$

$$\|\mathbb{A} \mathbf{v}\|^2 = (\mathbb{A} \mathbf{v})^\dagger \mathbb{A} \mathbf{v} = \mathbf{v}^\dagger \mathbb{A}^\dagger \mathbb{A} \mathbf{v} = \mathbf{v}^\dagger \mathbb{A} \mathbb{A}^\dagger \mathbf{v} = \|\mathbb{A}^\dagger \mathbf{v}\|^2$$

Therefore for any $c \in \mathbb{C}$

$$\|(\mathbb{A} - c \mathbb{1}) \mathbf{v}\|^2 = \|(\mathbb{A}^\dagger - c^* \mathbb{1}) \mathbf{v}\|^2$$

Hence choosing $\mathbf{v} = \mathbf{v}_k$ and $c = a_k$ yields

$$0 = \|(\mathbb{A}^\dagger - a_k^* \mathbb{1}) \mathbf{v}_k\|^2$$

□

Projectors

Before turning to the proof of the spectral theorem it is expedient to introduce the following

Definition. Projector. An operator $\mathbb{P}: \mathcal{H} \mapsto \mathcal{H}$ enjoying the following properties

- idempotency: $\mathbb{P}^2 = \mathbb{P}$
- identity on some $\tilde{\mathcal{H}} \subseteq \mathcal{H}$:

$$\mathbb{P} \mathbf{v} = \mathbf{v} \quad \forall \mathbf{v} \in \tilde{\mathcal{H}} \subseteq \mathcal{H}$$

- direct sum property: if $\tilde{\mathcal{H}}_\perp$ is the orthogonal complement of $\tilde{\mathcal{H}}$ then any vector $\mathbf{v} \in \mathcal{H}$ admits the decomposition

$$\mathbf{v} = \tilde{\mathbf{v}} + \tilde{\mathbf{v}}_\perp$$

where

$$\mathbb{P} \mathbf{v} = \tilde{\mathbf{v}} \quad \& \quad (\mathbb{1} - \mathbb{P}) \mathbf{v} = \tilde{\mathbf{v}}_\perp$$

We can associate to any unit vector \mathbf{u} in \mathcal{H} a projector \mathbb{P} by means of the **dual product** or column by row product

$$\mathbb{P} = \mathbf{u} \mathbf{u}^\dagger$$

Finally, if the collection of unit vectors $\{\mathbf{f}_i\}_{i=1}^d$ forms an orthonormal basis of the Hilbert space then the **completeness relation** is easy to verify

$$\sum_{i=1}^d \mathbb{P}_i \equiv \sum_{i=1}^d \mathbf{f}_i \mathbf{f}_i^\dagger = \mathbb{1}_d$$

holds true.

Proof of the spectral theorem

Theorem. Spectral decomposition. Any normal operator \mathbb{A} on a finite dimensional complex Hilbert space \mathcal{H} is diagonal with respect to some orthonormal basis for \mathcal{H} . Conversely, any diagonalizable operator is normal.

Proof.

Sufficient condition: if A is normal, it is amenable to diagonal form with respect to some orthonormal basis. Let a be an eigenvalue of A . In general we can write the projector onto the corresponding eigenspace in the form

$$\mathbb{P}_a = \sum_{k=1}^r \mathbf{v}_k \mathbf{v}_k^\dagger$$

where r is the degeneracy of a . Upon resorting to Gram-Schmidt orthonormalization we can always choose the \mathbf{a}_k 's such that

$$\mathbf{v}_i^\dagger \mathbf{v}_j = \delta_{ij} \quad (10)$$

It is readily seen that

$$\mathbb{P}_a = \mathbb{P}_a^\dagger \quad (11)$$

The projector to the space orthogonal to the a -eigenspace is then

$$\mathbb{Q}_a = \mathbb{1} - \mathbb{P}_a$$

since

$$\mathbb{Q}_a \mathbb{P}_a = (1 - \mathbb{P}_a) \mathbb{P}_a = \mathbb{P}_a - \mathbb{P}_a^2 = \mathbb{P}_a - \mathbb{P}_a = 0$$

and similarly $\mathbb{P}_a \mathbb{Q}_a = 0$. Independently of the assumption that \mathbb{A} be normal, we write

$$\mathbb{A} = (\mathbb{P}_a + \mathbb{Q}_a) \mathbb{A} (\mathbb{P}_a + \mathbb{Q}_a) = \mathbb{P}_a \mathbb{A} \mathbb{P}_a + \mathbb{P}_a \mathbb{A} \mathbb{Q}_a + \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a$$

since $\mathbb{Q}_a \mathbb{A} \mathbb{P}_a = 0$. Furthermore from $\mathbb{P}_a = \mathbb{P}_a^\dagger$ it follows that

$$\mathbb{P}_a \mathbb{A} \mathbb{Q}_a = (\mathbb{Q}_a^\dagger \mathbb{A}^\dagger \mathbb{P}_a^\dagger)^\dagger = (\mathbb{Q}_a \mathbb{A}^\dagger \mathbb{P}_a)^\dagger = (\mathbb{Q}_a a^* \mathbb{P}_a)^\dagger = a (\mathbb{Q}_a \mathbb{P}_a)^\dagger = 0$$

We therefore proved that

$$\mathbb{A} = \mathbb{P}_a \mathbb{A} \mathbb{P}_a + \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a$$

Obviously $\mathbb{P}_a \mathbb{A} \mathbb{P}_a$ is diagonal in the orthonormal basis of the \mathbf{v}_k 's spanning the a -eigenspace. To prove the claim it remains to show that $\mathbb{Q}_a \mathbb{A} \mathbb{Q}_a$ is normal in the subspace of \mathcal{H} orthogonal to the a -eigenspace. We verify that

$$\begin{aligned} \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a (\mathbb{Q}_a \mathbb{A} \mathbb{Q}_a)^\dagger &= \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a \mathbb{Q}_a \mathbb{A}^\dagger \mathbb{Q}_a = \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a \mathbb{A}^\dagger \mathbb{Q}_a \\ &= \mathbb{Q}_a \mathbb{A}^\dagger \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a = \mathbb{Q}_a \mathbb{A}^\dagger \mathbb{Q}_a \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a = (\mathbb{Q}_a \mathbb{A} \mathbb{Q}_a)^\dagger \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a \end{aligned}$$

Between the first and the second row we used

$$\begin{aligned} \mathbb{Q}_a \mathbb{A} \mathbb{Q}_a \mathbb{A}^\dagger \mathbb{Q}_a &= \mathbb{Q}_a \mathbb{A} (\mathbb{1} - \mathbb{P}_a) \mathbb{A}^\dagger \mathbb{Q}_a \\ &= \mathbb{Q}_a \mathbb{A} \mathbb{A}^\dagger \mathbb{Q}_a - \mathbb{Q}_a \mathbb{A} \mathbb{P}_a \mathbb{A}^\dagger \mathbb{Q}_a = \mathbb{Q}_a \mathbb{A} \mathbb{A}^\dagger \mathbb{Q}_a \end{aligned}$$

which holds since $\mathbb{Q}_a \mathbb{A} \mathbb{P}_a = 0$. Proceeding by induction we arrive at the representation of the normal matrix

$$\mathbb{A} = \sum_{i=1}^{n_a} a_i \sum_{j=1}^{r_i} \mathbf{v}_{j_i} \mathbf{v}_{j_i}^\dagger \quad (12)$$

where i counts the number of distinct eigenvalues and the j_1, \dots, j_{r_a} the elements of the basis spanning the eigenspace associated to a_i .

- **Necessary condition:** the converse follows from the observation that (12) is diagonal in the orthonormal basis of the eigenvectors of A . Representing these eigenvectors in a generic basis of \mathcal{H} yields a normal matrix. \square

One remark is in order

Remark. *The subspace associated to a degenerate eigenvalue a of a normal operator \mathbb{A} is spanned by a number of eigenvectors equal to the degeneracy n_a of the eigenvalue. Namely, if this were not the case there would exist a vector \mathbf{u} orthogonal to the eigenvectors \mathbf{v}_k with $k = 1, \dots, n_a$ such that*

$$\mathbb{A}\mathbf{u} = \sum_{k=1}^{n_a} c_k \mathbf{v}_k$$

But this hypothesis implies that

$$c_k = \mathbf{v}_k^\dagger \mathbb{A} \mathbf{u} = (\mathbb{A}^\dagger \mathbf{v}_k)^\dagger \mathbf{u} = a \mathbf{v}_k^\dagger \mathbf{u} = 0 \quad \forall k$$

Proposition. *If $\mathbb{A} = \mathbb{A}^\dagger$ the eigenvalues are real*

Proof. Let us label the eigenvalues by the index k eventually running over coinciding eigenvalues. Then

$$a_k = \mathbf{v}_k^\dagger \mathbb{A} \mathbf{v}_k = (\mathbb{A}^\dagger \mathbf{v}_k)^\dagger \mathbf{v}_k = (\mathbb{A} \mathbf{v}_k)^\dagger \mathbf{v}_k = a_k^*$$

\square

We can write generic operators in the Hilbert space as a linear combination of suitable self-adjoint operators

Proposition. *Any operator \mathbb{A} can be written in the form*

$$\mathbb{A} = \mathbb{R} + i \mathbb{I}$$

with

$$\mathbb{R}^\dagger = \mathbb{R} \quad \& \quad \mathbb{I}^\dagger = \mathbb{I}$$

In other words, a normal operator can always be represented in terms of a linear combination of two self-adjoint operators.

Proof. Under our hypotheses on the domain of definition of A it is immediate to observe that

$$\mathbb{R} = \frac{\mathbb{A} + \mathbb{A}^\dagger}{2} \quad \& \quad \mathbb{I} = \frac{\mathbb{A} - \mathbb{A}^\dagger}{2i}$$

\square

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