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# Algebraic Framework for Characterization of Mixed States in Quantum Computing Systems

by

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## Abstract

In this thesis, we introduce a unified algebraic framework in order to characterize mixed states, especially in the context of quantum computing systems. After a reminder of the fundamentals needed by the reader to better understand the use of mathematics as a quantum representation using three different but complementary approaches — Statistical, Algebraic,, and Geometric —.

To better understand this framework, we will apply those tools to the creation and analysis of quantum gates, error and noise correction codes, and quantum cryptology algorithms.

Moreover, concrete implementation and simulation (Qiskit, CIRQ) as well as experiments on IBM's Quantum Computer will allow us to put into practice concepts studied before.

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# I Introduction

## 1 Our position on the subject

Our main motivation to make this thesis was the idea that, despite being the foundation of the next big technological revolution, quantum mechanics and especially quantum computer engineering remain a rather abstract concept at first glance.

As such, we think the main issue of quantum mechanics is the lack of an intuitive and comprehensive framework to describe it, leading to too few people interesting themselves into it.

That is where algebra, as a mean of operating using comprehensive objects — such as matrices, vectors, etc —, became a prime candidate for a unified and accessible framework of quantum computing systems.

From these observations came our motivation in order to produce this thesis.

## 2 State of the Art

*“Quantum Computer : A computer that is based on the principles of quantum mechanics and uses qubits instead of bits. These computers are still in development and have the potential to solve complex problems much faster than conventional ones.”*

— Technical University of Munich’s Science Glossary (2025)

The history of quantum computers is the history of quantum mechanics itself. As soon as the idea of a parallel computing physic has been introduced, researchers thought about making computing systems out of them. And the most important part of these researches was the necessity to find a good way to represent what appeared as a succession of random and erratic phenomena. The idea to use algebraic means to characterize quantum states has been a prolific field of research since its introduction, as this is where operator theory, functional analysis, and quantum information science intersect. And while tentatives have been made in order to express those interactions solely by probabilistic means, a clear overview of complex systems using those has yet to be found. A mathematically well-established framework by means of operator algebras is hence of fundamental importance to theoretical modeling as well as to constructing trustworthy quantum computing devices.

Historically, the mathematization of quantum mechanics began by John Von Neumann’s contributions early in the 20th century, most of all by his classic book **"Mathematical Foundations**

**of Quantum Mechanics"** [27]. The introduction of the density matrix notion, along with its rigorous spectral theory, remains fundamental when distinguishing pure and mixed quantum states. His ideas were building blocks of what followed regarding C\*-algebras and constitute the backbone of today’s algebraic approach to quantum theory.

The theory of C\*-algebras, thoroughly delineated in reference texts such as Murphy’s "C-Algebras and Operator Theory" and Pedersen’s "C-Algebras and Their Automorphism Groups" , is a developed and robust framework for modeling observables of quantum mechanics. The invariant properties of operators — expressed through polynomial invariants such as trace, determinant, and higher-order traces — are effective means of exploring purity, entropy, and decoherence of quantum states. Such invariants are invariant under unitary conjugation, critical to maintaining that quantum processes are stable within computational contexts.

Use of these innovations within the context of quantum physics has been useful in developing the understanding of entanglement within quan-

tum systems. Moreover, Lie algebras, especially of the unitary groups, also have a crucial role to play in describing mechanics behind evolutions in quantum systems and remain a thriving subject of research. The **Baker-Campbell-Hausdorff formula** and **Casimir operator theory** supplement the set of algebraic means that can be brought to bear on analyzing quantum dynamics, providing finer insight into processes of coherence and decoherence. The synergy of operator algebraic means and Lie algebra is not only helpful to enhance the power of description of the framework but also opens up new directions of computational schemes of quantum error correction and circuit optimization.

Despite these well-established theoretical foundations, there are key challenges that remain. While invariant properties of density ma-

trices have been well studied, systematic application of those properties to characterize mixed states within real quantum computing devices is only emerging. Closing the gap between abstract algebraic formality and real quantum computational devices is therefore one of our key motivations here.

In summary, the subject of an algebraic characterization of mixed state is a variegated weave of mathematical disciplines ranging from early seminal work by *Von Neumann*, through C\*-algebra extensions, to the increasing importance of invariant theory and Lie algebras within quantum information science. While much has been done, much is yet to be accomplished to unlock full potential out of these algebraic resources in order to treat concrete issues of quantum computing.

### 3 Objectives of the thesis

Our objective by this thesis is to provide a complete and clear overview of the use of algebraic mean when working with multi-qubit quantum computing systems. As such, we pursue the following goals :

1. Provide a unified and explicit overview of the mathematical framework needed to understand quantum mechanic and especially a two-state quantum system — qubit —,
2. Interpret those fundamentals starting to simple quantum gates into more complex quantum circuits and systems,
3. Observe for ourselves our theory on measurement and noise by testing on actual quantum computers,

### 4 Methodology and Structure

The structure chosen for this paper follows a comprehensive and progressive evolution in order to fully grasp our subject. While Chapter II is more focused about giving the necessary definitions and properties for the later applications, Chapter III really introduce the concrete applications to quantum computers of theoretical objects seen before. As a way of verifying assertions made in past chapters, and give a real application to our researches, we also included a case study and experimental part in the form of Chapter IV by compiling and executing the Deutsch-Jozsa Algorithm on an actual quantum computer.

Our methodology has always been driven by the idea of linking abstract objects, properties and results to concrete and tangible physical object that anyone can observe for themselves.



## II Theoretical and Mathematical Foundations

### 1 Introduction to quantum states and representation

Sparked by *Max Planck*'s experiments of 1880-1900 on the "**Ultraviolet Catastrophe**"[11], the first objective of the emerging quantum theory was to find a formal description to a set of unresolved problems regarding blackbody radiation at shorter wavelengths. The singularity of this case led to the idea of a new branch of physics, bound not only by *Newtonian* gravitation theory or *Maxwell*'s electrostatics, but by something else yet to be discovered. This new field, confined to the subatomic realm and governed by its own distinct laws, quickly became a source of interest for European physicists and researchers.

As renowned physicists like *Albert Einstein* tried to find a way to include these anomalies into the standard determinist physic spectrum, concerned about its philosophical implications and believing that "*God does not play dice with the universe*"[12]. In fact, its behaviors appeared to be fundamentally erratic and unpredictable under existing tools. It then became crucial to identify strategies that allow physicists to forecast the behavior of such systems to carry out relevant experiments.

First formally introduced in 1925 by the German scientist *Werner Heisenberg* in his article "**Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen**" [*On the quantum-theoretical reinterpretation of kinematic and mechanical relationships*], this publication saw the idea of a new branch of physics called "*matrix mechanics*". This approach argued for an algebraic representation of quantum states, became the first mathematical framework to account for the uncertainty principle, and introduced the challenges of superposition and measurement uncertainty.

The beginning of the twentieth century saw the golden age of quantum theory of representation in Germany, with *Erwin Schrödinger*'s groundbreaking series of four articles in 1926, named "**Quantisierung als Eigenwertproblem**" [*Quantisation as eigenvalue problem*], proposing his idea of "wave mechanics".

*Schrödinger*'s work to oppose *Heisenberg*'s representation aimed to account for the wave-particle duality already theorized two years prior by *Louis de Broglie*'s wave experiment in 1924, who described without formalizing it how a subatomic corpus can act as either a wave or a particle depending on the context. In 1932, *John von Neumann* proposed the first axiomatic mathematical formulation of quantum states as linear operators in Hilbert spaces, deriving from functional analysis. In his book "**Mathematische Grundlagen der Quantenmechanik**" [*Mathematical Foundations of Quantum Mechanics*], *Von Neumann* also introduced the concept of pure and mixed states, depending on a system's interactions with its environment and observables.

The newly described density matrix allowed for the representation of quantum states in a more general way, taking into account both pure and mixed states by arranging them into a statistical mixture of pure states. This mathematical tool is crucial for analyzing the behavior of quantum machinery and designing efficient quantum algorithms.

For the purpose of this report, one should understand the properties and applications of the density matrix as the foundation for quantum computers and their upcoming evolution.

### 1.1 Pure and Mixed States

In order to understand Von Neumann's categorization of Quantum States, we first need to introduce ourselves to two cornerstones of modern quantum physics : the notion of **Hilbert space** and the **Bra-Ket notation**.

**Definition 1.1.1** We call **Hilbert space**  $\mathcal{H}$ , a complete inner-product space over  $\mathbb{C}$  which respects the following properties :

Let  $\langle x_1, x_2 \rangle$  be the scalar product of  $x_1, x_2$ , then,

1. **Linearity on the first term :**

$\forall x, y, z \in \mathcal{H}, \forall a, b \in \mathbb{C}$  we have :

$$\langle ax + by, z \rangle = a\langle x, z \rangle + b\langle y, z \rangle \quad (1.1.1)$$

2. **Anti-Linearity on the second term :**

$\forall x, y \in \mathcal{H}, \forall \lambda \in \mathbb{C}$  we have :

$$\langle x, \lambda y \rangle = \bar{\lambda} \langle x, y \rangle \quad (1.1.2)$$

3. **Conjugate symmetry :**

$\forall x, y \in \mathcal{H}$  we have :

$$\langle x, y \rangle = \overline{\langle y, x \rangle} \quad (1.1.3)$$

4. **Positive definiteness :**

$\forall x \in \mathcal{H}$  we have :

$$\langle x, x \rangle \geq 0 \quad (1.1.4)$$

And  $\langle x, x \rangle = 0 \implies x = 0$

5. **Completeness :**

Let  $(x_n)_{n \in \mathbb{N}}$  be a Cauchy sequence, then it converges to some  $x \in \mathcal{H}$  when  $n \rightarrow +\infty$ , this is equivalent to :

$$\lim_{n,m \rightarrow +\infty} \|x_n - x_m\| = 0, \implies x_n \rightarrow x \quad (1.1.5)$$

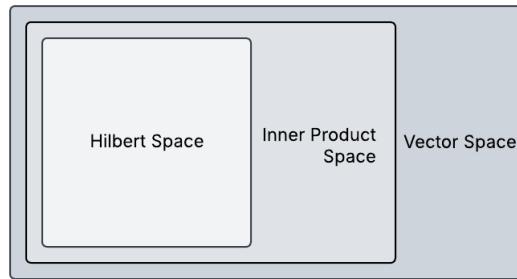


Figure 1.1: Hilbert Space Entanglement with Usual Spaces

**Definition 1.1.2** The **Bra-Ket notation** also called **Dirac's notation** from its inventor *Paul Dirac* is a compact way to represent quantum states, and linear operations on them, inside a defined Hilbert space, we then have :

1. Ket, denoted by  $|\psi\rangle$ , represent a column vector inside a Hilbert space  $\mathcal{H}$  and is used to describe the state of a quantum system.
2. Bra, denoted by  $\langle\psi|$ , represent the transposition of  $|\psi\rangle$  in the dual-space  $\mathcal{H}^*$ , and is useful to compute scalar product effectively.

**Example 1.1.3 :**  $|n\rangle$  is the pure state associated with the label  $n$

**Example 1.1.4 :**  $|\psi\rangle$  can also represent superposed states, for example, an ideal qu-bit can be written as a combination of pure states :

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Where  $\alpha, \beta \in \mathbb{C}$  and  $|\alpha|^2 + |\beta|^2 = 1$ , representing the probability amplitudes for outcomes 0 and 1 when observing  $|\psi\rangle$

**Example 1.1.5 :** If we set  $|\psi\rangle = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ , we then have :

$$\langle\psi| = (\bar{x}_1 \ \bar{x}_2)$$

Where  $\bar{x}_1$  and  $\bar{x}_2$  represent the **complex conjugate** of respectively  $x_1$  and  $x_2$ .

**Definition 1.1.6** Let  $|\psi_1\rangle, |\psi_2\rangle$  be two vector-columns inside a Hilbert Space  $\mathcal{H}$ , then we call **complex scalar product** of  $|\psi_1\rangle, |\psi_2\rangle$  the application  $\langle\psi_1|\psi_2\rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$  such that:

$$\langle\psi_1|\psi_2\rangle = \sum_i \overline{\psi_1}(i) \psi_2(i) \quad (1.1.6)$$

Where  $\overline{\psi_1}(i)$  is the  $i$ -th complex conjugate of  $|\psi_1\rangle$ , and  $\psi_2(i)$  the  $i$ -th composant of  $|\psi_2\rangle$ .

**Properties 1.1.7** Let  $|\psi_1\rangle, |\psi_2\rangle, |\phi\rangle \in \mathcal{H}$  and  $a, b \in \mathbb{C}$  :

**1. Complex Conjugation**

$$\langle\psi_1|\psi_2\rangle = \overline{\langle\psi_2|\psi_1\rangle} \quad (1.1.7)$$

**2. Linearity of Ket & Anti-Linearity of Bra**

$$\langle\phi|(a|\psi_1\rangle + b|\psi_2\rangle) = a\langle\phi|\psi_1\rangle + b\langle\phi|\psi_2\rangle \quad (1.1.8)$$

$$(a\langle\psi_1| + b\langle\psi_2|)|\phi\rangle = \bar{a}\langle\psi_1|\phi\rangle + \bar{b}\langle\psi_2|\phi\rangle \quad (1.1.9)$$

**4. Norm of the Product**

$$\langle\psi|\psi\rangle = \|\psi\|^2 \geq 0 \quad (1.1.10)$$

And  $\langle\psi|\psi\rangle = 0 \iff \psi = 0$

**Definition 1.1.8** A Quantum State  $|\phi\rangle$  is called **Pure** if and only if it can be fully represented by a unit vector  $|\psi\rangle$  and such that  $\langle\psi|\psi\rangle = 1$ , this property implies that the distribution of its internal states are coherent and can be fully described by a single object.

### Properties 1.1.9

**1. Quantum measurement** If we have a pure quantum state, Then

$$|\psi\rangle = \sum_i a_i |i\rangle \quad (1.1.11)$$

Moreover, probability of obtaining outcome  $|i\rangle$  upon measurement is given by  $P(|i\rangle) = |a_i|^2$ .

**2. Phase** Let  $|\psi\rangle$  be a pure state, then we have :

$$|\psi\rangle = e^{i\theta} |\psi\rangle \quad (1.1.12)$$

This implies that a pure state is not global-phase dependent, but actually, if we set  $|\psi\rangle$  such that :

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle + e^{i\theta} |1\rangle) \quad (1.1.13)$$

Then the phase  $\theta$  determine the interference effect.

**3. Entropy** Let  $S$  denote the classical Von Neumann's entropy, and let  $|\psi\rangle$  be a pure state. Then we have :

$$S(|\psi\rangle) = 0 \quad (1.1.14)$$

This implies the lack of classical uncertainty.

**Definition 1.1.10** A Quantum State  $|\phi\rangle$  is called **Mixed** if its not Pure, hence, if his distribution is incoherent and can only be describe as a statistical mixture of pure states. We will look more into the specific representation of mixed states and their implications in [Part 1.2](#).

### Properties 1.1.11

**1. Quantum Measurement** The probability  $P$  of measuring  $i$  while observing a mixed state represented by its **density matrix**  $\rho$  is :

$$P(i) = \text{Tr}(\rho M_i) \quad (1.1.15)$$

Where  $M_i$  is the  $i$ -th **operator** (mathematical representation of the measurement process) i.e., the interaction between a quantum system and an **observator**.

**2. Entropy** Let  $S$  denote the classical Von Neumann's entropy, and let  $\rho$  the density matrix of a mixed state  $|\psi\rangle$ . Then we have :

$$S(\rho) = -\text{Tr}(\rho \log \rho) > 0 \quad (1.1.16)$$

This implies the inherence of uncertainty to mixed states.

## 1.2 Wave Mechanics Vs Matrix Mechanics

Now that we saw those basic definitions, we can start looking inside *Schrödinger's Wave Mechanic* and *Heisenberg's Matrix Mechanic* in order to choose which one is the most suitable for a **discrete application**. It is first important to note that *Von Neumann* mathematically proved those two approaches as equivalent. As such, we will talk more about "**Wave representation**" and "**Matricial representation**" as they both describe the same mechanical phenomena.

**Definition 1.2.1 — Schrödinger's Equation.** *Schrödinger* chooses to consider the evolution of quantum states through time while fixing the operators, this system leads to a continuous representation described by the following equation :

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (1.2.1)$$

Where  $\hat{H}$  is the Hamiltonian operator (i.e. the total energy of the system) and  $\hbar$  the reduced Planck's constant.

**Remark 1.2.2** Here,  $|\psi(t)\rangle$  represent the probability of finding a particle in the  $\psi$  state at time  $t$  and not a particle itself. Also, while this equation is useful to quantify continuous systems, it becomes too heavy for a **discrete application**, especially for **mixed states**.

**Definition 1.2.3 — Heisenberg's Equation.** Contrary to *Schrödinger*, *Heisenberg* considered the quantum states to be fixed and materialize the evolution of the operators through time. This equation became the first clear bridge between algebra and quantum physics using his own equation, stated as :

$$\frac{d\hat{A}_H(t)}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{A}_H(t)] + \frac{\partial \hat{A}_H(t)}{\partial t} \quad (1.2.2)$$

Where  $\hat{H}$  is the Hamiltonian operator and  $\hat{A}_H(t)$  the fluctuating operator.

**Remark 1.2.4** This representation is better and more intuitive for a **discrete application** but still lack clarity and methods when representing **mixed states**.

**Remark 1.2.5 — Von Neumann's necessary opening.** When those representation were good complementary computation techniques for systems of pure states, it became clear that they lacked a satisfying way to represent and interpret mixed states. Von Neumann's idea to use a density matrix allowed to generalize the description of quantum system, as an algebraic and statistics intricate to include both type of state.

**Definition 1.2.6** Let  $\rho$  denote the **density matrix** of a quantum state  $|\psi\rangle$  :

1. The algebraic representation of a **pure state** depending on time  $t$  is given by :

$$\rho(t) = |\psi(t)\rangle \langle \psi(t)| \quad (1.2.3)$$

2. The statistics representation of a **mixed state** is therefore :

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)| \quad (1.2.4)$$

Where  $p_i \in [0, 1]$  represent the probability distribution of  $|\psi_i(t)\rangle \langle \psi_i(t)|$

**Definition 1.2.7** We call **trace** of a matrix  $\rho$  the sum of its diagonal elements :

$$\text{Tr}(\rho) = \sum_{i=1}^n \rho_{ii} \quad (1.2.5)$$

Where  $\rho_{ii}$  correspond to the element of coordinates  $(i, i)$  in  $\rho$ .

### Properties 1.2.8

**Trace of a pure state matrix** Let  $\rho$  the density matrix representing a pure state  $|\psi\rangle$ , then we have :

$$\text{Tr}(\rho) = 1 \quad (1.2.6)$$

Moreover,

$$\text{Tr}(\rho^2) = \sum_{i=1}^n \rho_{ii}^2 = 1 \quad (1.2.7)$$

This property represent the coherence and certainty of the state  $|\psi\rangle$ .

**Trace of a mixed state matrix** Let  $\rho$  the density matrix representing a mixed state  $|\psi\rangle$ , then we have :

$$\text{Tr}(\rho) = 1 \quad (1.2.8)$$

Moreover,

$$\text{Tr}(\rho^2) = \sum_{i=1}^n \rho_{ii}^2 < 1 \quad (1.2.9)$$

This represent the incoherent probabilistic distribution of the state  $|\psi\rangle$ . This property can be proved using the Cauchy-Schwarz inequality :

$$|\langle\psi_1|\psi_2\rangle| \leq \|\psi_1\| \cdot \|\psi_2\|, \text{ and } |\langle\psi_1|\psi_2\rangle| = \|\psi_1\| \cdot \|\psi_2\| \iff \exists \lambda \in \mathbb{C} \mid |\psi_1\rangle = \lambda|\psi_2\rangle$$

As only pure states are linearly dependent one to another, we have  $\text{Tr}(\rho) < 1$  [28, section 2.4.2]. This property of mixed state illustrate the —incoherent— statistical preparation of those states.

**Example 1.2.9 — The ideal Qubit** Let  $|0\rangle$  and  $|1\rangle$  be two pure states represented by their density matrix respectively  $\rho(|0\rangle) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix}$ ,  $\rho(|1\rangle) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix}$ . And let  $\alpha, \beta \in \mathbb{R}$ , s.t.  $|\alpha|^2 + |\beta|^2 = 1$ , then we can represent the qubit  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  as :

$$\rho(|\psi\rangle) = |\psi\rangle\langle\psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}\begin{pmatrix} \bar{\alpha} & \bar{\beta} \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha\bar{\beta} \\ \bar{\alpha}\beta & |\beta|^2 \end{pmatrix}$$

Here we can see that the *ideal* model of a Qu-bit is a superposed **pure** state as its trace  $\text{Tr}(\rho(|\psi\rangle)) = |\alpha|^2 + |\beta|^2 = 1$ .

**Example 1.2.10 — The practical Qubit** In reality, multiple interference in the system can impact the purity of the states, as such, it is in practice almost impossible to reach  $\text{Tr}(\rho) = 1$ , making the whole system **incoherent**. A global representation of this phenomenon is the Bloch's Sphere that we will study in greater depth in [part 2.4](#)

### 1.3 Superposition and Entanglement

*“Entanglement is one of the most fundamental resources for quantum information processing.”*

— Horodecki, R., Horodecki, P., Horodecki, M. & Horodecki, K. (2009)

**Definition 1.3.1** A quantum state can exist simultaneously as multiple base states. This notion is defined by the **Superposition Principle**[28], stating that any  $|\psi\rangle \in \mathcal{H}$  can be described as a linear combination of  $|\phi_i\rangle \in \mathcal{H}$  :

$$|\psi\rangle = \sum_{k=1}^n \alpha_k |\phi_k\rangle \quad (1.3.1)$$

Where  $\alpha_i \in \mathbb{C}$  represent the complex coefficient of  $\phi_i$  and  $\sum_{k=0}^n |\alpha_k|^2 = 1$  (following [properties 1.2.7](#))

**Remark 1.3.2** This definition come directly from the linearity of Hilbert Space.

**Remark 1.3.3** As  $\alpha_i$  are complex coefficient, they can also interact in a negative or destructive way. This allows us to use a linear combination to represent noises and interferences inherent to applied quantum system.

**Property 1.3.4 — Linear Evolution and Conservation of Superposition** Let  $|\psi(t)\rangle \in \mathcal{H}$  be a quantum state, suppose  $\mathcal{H}$  be without exterior perturbations. Then by previous definition, we have :

$$|\psi(t_0)\rangle = \sum_{k=0}^n \alpha_k |\phi_k\rangle \quad (1.3.2)$$

Then the global state  $|\psi(t)\rangle$  for any  $t$  can be defined as :

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle = U(t, t_0) \sum_{k=0}^n \alpha_k |\phi_k\rangle = \sum_{k=0}^n U(t, t_0) \alpha_k |\phi_k\rangle \quad (1.3.3)$$

Where  $U(t, t_0)$  is a unitary linear operator that preserve superposition and the condition  $\sum |\alpha_i|^2 = 1$ .

**Definition 1.3.5** A composite quantum state  $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$  is called **entangled** if it cannot be represented as a [tensor products](#) of unitary elements.

This implies that for all  $|\phi_1\rangle$  and  $|\phi_2\rangle$  being two states in respectively  $\mathcal{H}_1$  and  $\mathcal{H}_2$ . Then,

$$|\psi\rangle \neq |\phi_1\rangle \otimes |\phi_2\rangle \quad (1.3.4)$$

**Property 1.3.6** Following the same principle as superposition, entangled states in an isolated system conserve their status through time evolution. [18]

**Remark 1.3.7** Entanglement and its quantification represent a cornerstone of applied quantum computing systems. Despite the development of various measures such as entanglement entropy, negativity, or concurrence, the phenomenon of entanglement remains a subject of debate regarding the completeness of quantum physics. [12]

## 1.4 Linear Operators

**Definition 1.4.1** Let  $A$  be an application on a Hilbert Space  $\mathcal{H}$ , then,  $A$  is a **linear operator** if  $\forall \alpha, \beta \in \mathbb{C}$  and  $\forall |\psi\rangle, |\phi\rangle \in \mathcal{H}$ . We have the following property :

$$A(\alpha|\psi\rangle + \beta|\phi\rangle) = A\alpha|\psi\rangle + A\beta|\phi\rangle \quad (1.4.1)$$

**Definition 1.4.2** Let  $A$  be a linear operator on  $\mathcal{H}$ , we denote by  $A^\dagger$  the **adjoint operator** of  $A$ . Moreover,  $A^\dagger$  is the unitary operator satisfying the following equation :

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

$$\langle \psi | A | \phi \rangle = \langle A^\dagger \psi | \phi \rangle \quad (1.4.2)$$

**Definition 1.4.3** Let  $A$  be a linear operator on  $\mathcal{H}$ ,  $A$  is called **hermitian** if and only if we have :

$$A = A^\dagger \quad (1.4.3)$$

**Property 1.4.4** Moreover, let  $A$  be a hermitian map and  $\langle \cdot, \cdot \rangle$  the usual scalar product on  $\mathbb{C}^n$ . Then,  $\forall x, y \in \mathcal{H}$  we have :

$$\langle Ax, y \rangle = \langle x, Ay \rangle \quad (1.4.4)$$

**Remark 1.4.5** Hermitian operators are of significant use in quantum computations : Hermitian operators are used to represent physical observables and are fundamental for the **theory of spectral decomposition** that we will see in depth in **part 2.2**.

**Opening 1.4.6** Those definitions and properties represent a solid basis for us to study quantum states and systems; for that, we will now see more complex system representations using different fields of mathematics and compare them for our use case in the context of quantum computer networks.

## 2 Modern Mathematical Representation of Quantum States

### 2.1 Statistical Approach

**Definition 2.1.1** In the first part, we talked about Schrödinger's Equation without properly introducing the idea of a wave function  $\psi(\vec{r}, t)$ , where  $\psi$  is a complex continuous function of the space variable  $\vec{r} = (x, y, z)$

This function represent the complete description of the state of a particle at an instant  $t$

**Remark 2.1.2** When we say that the description made by the wave function is complete, we imply that there is no other element that could make it possible to know before the measurement, where the particle is going to be detected.

*The probabilistic and random character of this framework is not due to a poor knowledge of the initial conditions (as in the kinetic theory of gases, for example). But is the main focus of quantum formalism.*

**Properties 2.1.3** The wave function is called "probability amplitude" and as such, we can link it to a probability law such that  $d^3P = |\psi(\vec{r}, t)|^2 d^3r$  represent the probability of finding the particle at time  $t$  in the volume  $d^3r$  surrounding  $\vec{r}$ .

We set the following constraint :

$$\int |\psi(\vec{r}, t)|^2 d^3r = 1 \quad (2.1.1)$$

i.e. the probability law is normalized, hence we can apply the usual probability functions to  $P$  :

1. The mean position of  $x$  denoted by  $\langle x \rangle$  is defined by :

$$\langle x \rangle = \int x |\psi(x)|^2 dx \quad (2.1.2)$$

2. The variance  $\Delta x^2$  is :

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2 \quad (2.1.3)$$

3. Therefore the standard deviation  $\Delta x$ , defined as the square root of the variance is :

$$\Delta x = \sqrt{\Delta x^2} \quad (2.1.4)$$

**Property 2.1.4** Those properties also allow us to represent superposed states and interference : If  $\psi_1$  and  $\psi_2$  are two wave functions with probability laws  $P_1 = |\psi_1|^2$ ,  $P_2 = |\psi_2|^2$ , then :

$$\psi \propto \psi_1 + \psi_2 \quad (2.1.5)$$

And the corresponding probability law  $P$  is :

$$P = |\psi|^2 \propto P_1 + P_2 + \underbrace{\psi_1 \bar{\psi}_2 + \bar{\psi}_1 \psi_2}_{\text{interferences}} \quad (2.1.6)$$

**Remark 2.1.5** While this approach corresponds well to the results found by experiments, it still lacks depth regarding non-commutative operations, dynamic transforms, and any kind of error correction inside quantum computers. Overall, while representing a good starting point, we still need to introduce more flexible types of objects in order to better manipulate quantum states.

## 2.2 Algebraic Approach

**Definition 2.2.1** We call  $A$  a **C\*-Algebra**, a Banach algebra in  $\mathbb{C}$  ruled by a map  $x \mapsto x^*$  using the following properties [14]:

Let  $x, y \in A$ ,  $\lambda \in \mathbb{C}$  and  $e$  be the neutral element of  $A$  (here 1):

1. It is an involution :

$$(x^*)^* = x^{**} = x \quad (2.2.1)$$

2. Distribution :

$$\begin{aligned} (x + y)^* &= x^* + y^* \\ (xy)^* &= y^* x^* \end{aligned} \quad (2.2.2)$$

3. Scalar conjugaison :

$$(\lambda x)^* = \bar{\lambda} x^* \quad (2.2.3)$$

4. Norm product :

$$\|x\| \|x^*\| = \|x^* x\| = \|x\|^2 = \sup\{|\lambda| : x^* x - \lambda e \text{ not invertible}\} \quad (2.2.4)$$

**Theorem 2.2.2 — Gelfand–Naimark theorem** The Gelfand–Naimark theorem is fundamental to understanding the usefulness of C\*-Algebra in quantum computations as it links operators on Hilbert Space with abstract Algebraic representation. And is formulated as follows :

Let  $A$  a be a  $C^*$ -Algebra, and let  $\mathcal{H}$  be a Hilbert Space. Then, there exists  $\pi(x)$  a \*-isomorphic application such that :

$$\pi : A \rightarrow B(\mathcal{H}) \quad (2.2.5)$$

With  $B(\mathcal{H})$  the set of bounded operators of  $\mathcal{H}$ .

This implies that for any  $L \in B(\mathcal{H})$ , we have :

$$\exists M > 0, \forall x \in \mathcal{H} \mid \|Lx\| \leq M \|x\| \quad (2.2.6)$$

Moreover,

1.  $\forall a \in A, \|\pi(a)\| = \|a\|$
2.  $\pi$  is injective and preserve all algebraic operations

This theorem shows that any abstract  $C^*$ -Algebra object can be transformed into an measurable and concrete object inside a Hilbert Space; moreover, the preservation of norms and \*-structure play a fundamental role when describing a system's stability.

An application of this principle will be seen in-depth in [Theorem 2.2.10](#) and is the key in concrete uses of theorems and properties seen in this chapter.

**Definition 2.2.4 — Von Neumann’s Algebra [10], [37]**

Von Neumann’s algebra, also sometimes called  $W^*$ -Algebra, is a specific sub-type of  $C^*$ -Algebra. Hence, the previous properties and theorem we saw also apply here.

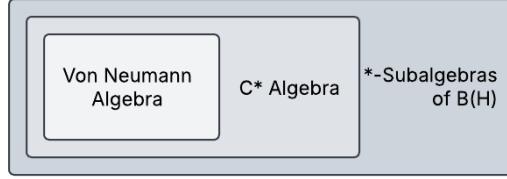


Figure 2.1: Global Intrication of Studied Algebras

As such, Von Neumann’s algebra act as a more restrictive framework while preserving the Gelfand–Naimark theorem and its usefulness in quantum computations.

The formal definition from Von Neumann implies introduction multiple topological concepts. Therefore, for the sake of this thesis we will resume it to its fundamental properties for quantum computing systems.

**Properties 2.2.5****1. Stability of the limit**

Let  $W$  be a Von Neumann Algebra, then  $\forall(M_n) \in W$  a sequence of operators in  $W$ , we have :

$$\lim_{n \rightarrow \infty} M_n = l \quad (2.2.7)$$

then  $l \in W$

This ensure that any limit of operators in  $W$  is still within  $W$ .

**2. Von Neumann bicommutant theorem**

Let  $W$  be a Von Neumann Algebra, then, we have :

$$W = W'' \quad (2.2.8)$$

Where  $W'$  is the set of all bounded operators that commute with every element of  $W$

**Remark 2.2.6 The necessity of Von Neumann’s  $C^*$ -algebra restriction**

The introduction of Von Neumann algebra compared to standard  $C^*$ -algebra allow us the expand our reach beyond finite quantum system. Its properties are the basis of quantum field theory and statistical mechanics. These properties form the cornerstone of non-commutative measure theory, providing powerful tools to define and analyze quantum observables, states, and measurement processes.

**Property 2.2.7 — Linear Operations**

**Definition 2.2.8** We call **Spectrum** of  $A$ , denoted by  $\sigma(A)$ , the set of its eigenvalues on  $\mathcal{H}$ .

**Remark 2.2.9 — Application to quantum perspective**

Let  $\sigma(A) = \{\lambda_1 \rightarrow \lambda_n\}$ , then  $\lambda_i$  is the  $i$ -th possible outcome of  $A$ .

Hence, the spectrum of an operator  $A$  represent all the possible measures obtained when observing  $A$ .

**Theorem 2.2.10 — Spectral Theory of Decomposition[32]**

*This theorem and its applications are the back spine of this thesis at it is what allow us the the matrix efficiently in order to analyses quantum systems and therefore apply those to computing systems*

Let  $A$  be a bounded self-adjoint operator acting on  $\mathcal{H}$ ,

Then, there exists a family of orthogonal projections, indexed by  $\sigma = \sigma(A)$  the spectrum of  $A$ ,

We denote this set by  $\{E(\lambda)\}, \lambda \in \sigma$  such that the following property is true :

$$A = \int_{\sigma} \lambda dE(\lambda) \quad (2.2.9)$$

This implies that any operator  $A$  can be continuously diagonalized as their outcomes  $\lambda$ , weighted by the corresponding projectors

**Property 2.2.11 — Application of the theorem** This theorem is crucial when applied to quantum computers, as it is what allows for fast computation of the evolution of a system, denoted by  $U_A(t)$  and defined by  $e^{-iAt}$ :

$$U_A(t) = e^{-iAt} = \text{by theorem 2.2.10} \int_{\sigma(A)} e^{-i\lambda t} dE(\lambda) \quad (2.2.10)$$

This is especially useful as we know how to compute such integrals easily.

Moreover, the spectral theory of decomposition allows us to study each outcome independently and to produce a statistical overview of the system without the usual problems concerning entanglement and mixed states that would have been encountered if we only worked with statistical properties.

**Definition 2.2.12 — Partial Trace and Reduced Density Matrix** [25] Let  $\mathcal{H}_1$  and  $\mathcal{H}_2$  be two Hilbert spaces associated with their own quantum system. Let their global composite system described by the tensor product  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ . Let  $\rho$  be a density matrix over  $\mathcal{H}$ ,

we call **Partial Trace** over  $\mathcal{H}_2$  — denoted  $\text{Tr}_{\mathcal{H}_2}$  — the operation such that :

$$\rho_1 = \text{Tr}_{\mathcal{H}_2}(\rho) \quad (2.2.11)$$

Where  $\rho_1$  is called **reduced density matrix** on  $\mathcal{H}_1$

**Remark 2.2.13** This definition yields the degrees of liberty associated with  $\mathcal{H}_2$  provided with  $\mathcal{H}_1$ . This definition allows us to accurately describe any measurements made on a subsystem  $\mathcal{H}_1$  of  $\mathcal{H}$  using solely  $\rho_1$  for any observable  $O$  on  $\mathcal{H}_1$ .

Even more, this definition allows us to compute the expected value of such system as :

$$\text{Tr}_{\mathcal{H}_1}(O\rho_1) = \text{Tr}_{\mathcal{H}}(O \otimes I_2\rho) \quad (2.2.12)$$

Where  $I_2$  is the identity matrix over  $\mathcal{H}_2$ .

*Examples for this part and more in-depth correction can be found in R. LaRose Seminar Notes's exercices [23]*

**Example 2.2.14** Partial Trace of Pure States Product

Let  $|\psi\rangle$  be a composite of pure state over  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ ,  $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ . And ruled by a density matrix  $\rho$  such that,  $\rho = |\psi\rangle\langle\psi| = |\psi_1\rangle\langle\psi_1| \otimes |\psi_2\rangle\langle\psi_2|$ ,

Then, the reduced density matrix  $\rho_1$  of  $|\psi_1\rangle$  over  $|\psi_2\rangle$  is :

$$\rho_1 = \text{Tr}_{\mathcal{H}_2}(\rho) = |\psi_1\rangle\langle\psi_1| \times \underbrace{\text{Tr}(|\psi_2\rangle\langle\psi_2|)}_{=1 \text{ as } |\psi_1\rangle \text{ is a pure state}} = |\psi_1\rangle\langle\psi_1| \quad (2.2.13)$$

This allows us to confirm the purity of  $|\psi_1\rangle$  as its reduced density matrix  $\rho_1$  is still pure when traced over  $|\psi_2\rangle$ .

**Example 2.2.15** Partial Trace of Entangled States

Let  $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$  be the maximally entangled Bell state of a two-qubits system, with two subsystems  $|\Phi_1^+\rangle, |\Phi_2^+\rangle$  each representing a qubits over respectively  $\mathcal{H}_1, \mathcal{H}_2$ . Hence, for  $i, k \in \{0, 1\}$ , we have :  $|ik\rangle = |i\rangle_{\mathcal{H}_1} \otimes |k\rangle_{\mathcal{H}_2}$ .

We set  $\rho$  the density matrix of the system as :

$$\rho = |\Phi^+\rangle\langle\Phi^+| = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \quad (2.2.14)$$

Then,  $\rho_{\mathcal{H}_1}$  is :

$$\rho_{\mathcal{H}_1} = \text{Tr}_{\mathcal{H}_2}(\rho) = \langle 0_{\mathcal{H}_2} | \rho | 0_{\mathcal{H}_2} \rangle + \langle 1_{\mathcal{H}_2} | \rho | 1_{\mathcal{H}_2} \rangle = \frac{1}{2}(|0_{\mathcal{H}_1}\rangle\langle 0_{\mathcal{H}_1}| + |1_{\mathcal{H}_1}\rangle\langle 1_{\mathcal{H}_1}|) \quad (2.2.15)$$

Therefore,  $\rho_{\mathcal{H}_1} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2}I_{|\Phi_1^+\rangle}$ , with  $I_{|\Phi_1^+\rangle}$  being the identity matrix of  $|\Phi_1^+\rangle$

### 2.3 Example of Geometrical representation

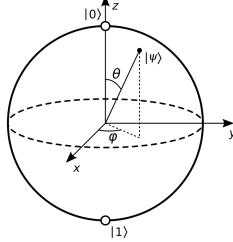


Figure 2.2: Usual Bloch's Sphere Representation[34]

**Principle 2.3.1[28]** Let a standard two-level quantum system ( $|\psi\rangle$  qubit system), we saw that any pure quantum state can be decomposed as a sum of the basis vectors  $|0\rangle, |1\rangle$  and a corresponding complex number  $\alpha, \beta$ . Moreover, we saw that the total probability of outcomes of a system  $\langle\psi|\phi\rangle$  is always 1.

This property allows for pure states to be described by only three real numbers, giving rise to the idea of a 3-dimensional representation — Bloch's Sphere — using the following idea :

$$|\psi\rangle = \left[ \cos\left(\frac{\theta}{2}\right) |0\rangle \right] + \left[ \cos(\phi) + i \sin(\phi) \sin\left(\frac{\theta}{2}\right) |1\rangle \right] \quad (2.3.1)$$

Where  $0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi$ ,

Those coordinates give use a **unique** point on the surface of the sphere (as  $\| |\psi\rangle \| = 1$ ), for any pure quantum state.

On the other hand, mixed states can still be described using their density matrix  $\rho$ :

$$\begin{aligned} \rho &= \frac{1}{2}(I + \vec{a} \times \vec{\sigma}) = \frac{1}{2} \left[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + a_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + a_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \\ &= \frac{1}{2} \begin{pmatrix} 1 + a_z & a_x - ia_y \\ a_x + ia_y & 1 - a_z \end{pmatrix} \end{aligned} \quad (2.3.2)$$

Where  $\vec{\sigma}$  is a Pauli matrix (complex, traceless, Hermitian, involutory, and unitary), We call  $\vec{a} = (\vec{a}_x, \vec{a}_y, \vec{a}_z) \in \mathbb{R}^3$  a Bloch vector, with  $a_x, a_y, a_z$  being the unique coordinates of the related quantum state inside Bloch's sphere — that we call Bloch's Ball when considering also mixed quantum states-.

This representation allows us to visually determine that, due to their incoherent nature, the total probability  $|\vec{a}|$  of a mixed system is **less or equal to 1**. Hence allowing it to be placed below the sphere's surface.

**Usefulness** This intuitive representation is great for giving a unitary and comprehensive overview of a two-state quantum system such as qubits. Furthermore, the concept of the Bloch sphere can be extended beyond two dimensions, making it applicable to more complex quantum systems.

**Acknowledgment** We extensively utilized Konstantin Herb's Bloch sphere simulator [17] to visualize and better understand the dynamics discussed in this section.

## 2.4 Entropy, Decoherence and Interference

In part 1.3 with property 1.3.4 and 1.3.6, we saw that isolated systems conserve superposition and entanglement. mini intro partie

### Definition 2.4.1 — Von Neumann Entropy [27][3]

Let  $\rho$  be the density matrix of a quantum system  $|\psi\rangle$  on  $\mathcal{H}$ , we call **Von Neumann Entropy**, denoted by  $S$ , the statistical uncertainty within a description of  $|\psi\rangle$  :

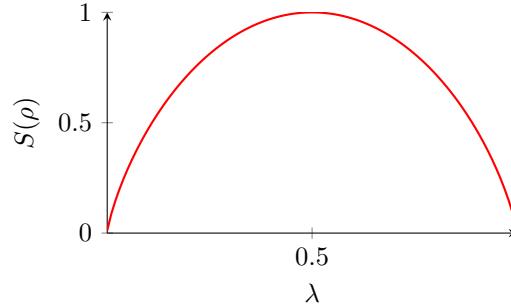
$$S = -\text{Tr}(\rho \ln \rho) \quad (2.4.1)$$

### Properties 2.4.2

1.  $S(\rho) = 0 \iff |\psi\rangle$  is a pure state.
2.  $S(\rho)$  is maximal for a maximally mixed state, i.e  $\rho = \frac{1}{2}I$ .
3.  $S(\rho)$  is symmetric with respect to  $\lambda = \frac{1}{2}$ .
4.  $S(\rho)$  is concave on  $[0, 1]$ .
5.  $S(\rho)$  is additive for two independent systems  $A, B$  :

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B) \quad (2.4.2)$$

Let  $\rho = \begin{pmatrix} \lambda & 0 \\ 0 & 1-\lambda \end{pmatrix}$ , then we can plot a 2 dimensional Von Neumann Entropy following properties seen above :



**Remark 2.4.4 — Entropy and Measurement** Let  $E_i$  be a positive operator-valued measure (POVM), where each  $E_i$  is a positive semi-definite operator such that  $\sum E_i = I$ . A quantum measurement described by this POVM can be implemented via a set of Kraus operators  $A_i$  satisfying:

$$E_i = A_i^\dagger A_i \quad (2.4.3)$$

If the measurement outcome  $i$  is obtained, the post-measurement state becomes:

$$\rho \rightarrow \rho' = \frac{A_i \rho A_i^\dagger}{\text{Tr}(\rho E_i)} \quad (2.4.4)$$

This process generally increases the entropy of the system, as it corresponds to a partial loss of quantum information due to entanglement with the measurement.

**Definition 2.4.4 — Decoherence** Let a quantum system  $|\psi\rangle$  over  $\mathcal{H}$ , and  $\rho$  its density matrix. **Decoherence** refers to the process by which quantum superpositions in  $|\psi\rangle$  are dynamically suppressed due to entanglement with an environment E resulting in the apparent emergence of classical probabilistic behavior[40].

In practice, Decoherence manifests as the decay of off-diagonal elements (coherence) in  $\rho$  when expressed in the "pointer basis". This suppression of coherence leads to the rationalization of the system's behavior.

**Example 2.4.6** Let  $|\psi(t)\rangle$  be the time  $t$  evolution of two-level quantum system, with a thermal environment  $T$ .

Let  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle; \alpha, \beta \in \mathbb{C}$  and defined by its density matrix  $\rho(t)$ . Then the interaction can be modeled by a Lindblad equation (generalization of Schrödinger Equation to open systems) such that :

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H, \rho(t)] + \sum_k \left( L_k \rho(t) L_k^\dagger - \frac{1}{2} \{ L_k^\dagger L_k, \rho(t) \} \right) \quad (2.4.5)$$

Where  $H$  is the Hamiltonian of the system (reminder : the total energy), and  $L_k$  are called Lindblad operators and represent the dissipation effect applied over the system[5].

**Property 2.4.7** In quantum mechanics, interference arises from the coherent superposition of states. Decoherence, by suppressing off-diagonal elements in the system's density matrix, diminishes the ability of the system to exhibit interference effects.[8]

**Remark 2.4.8** Decoherence is intrinsically linked to the concept of entropy in quantum systems. As a system de-coheres due to environmental interactions. Moreover, this behavior tend to increase Von Neumann Entropy of the system reflecting the loss of information about the system.

**Definition 2.4.9 — Interference** We call **Interference** the interaction between superposed states inside a quantum system  $|\psi\rangle$ . This interaction can be either constructive or destructive depending their respective momentum. This property is especially visible in Young's Double-slit experiment where bright lines represent constructive interference —boosting the energy of a wave—, while dark lines arise from destructive behavior —two waves canceling each other—.

#### Example 2.4.10 — Mach-Zehnder Interferometer

The Mach-Zehnder Interferometer serves as a simplified version of Young's double-slit experiment, utilizing lasers and half-silvered mirrors to study interference patterns. It splits a beam of light into two paths, introduces a phase shift in one path, and then recombines them to observe constructive or destructive interference based on the relative phase difference.

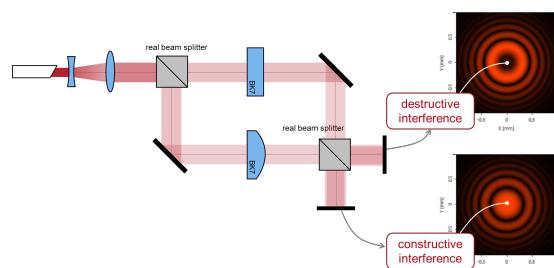


Figure 2.3: Interferometer setup [24]

### 3 Introduction to Tensor Product

At multiples instances during this first part, we mentioned an operation denoted by  $\otimes$  — for example as  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$  in [Definition 2.2.12](#) —, without explicitly giving a definition and properties associated with it.

The goal of this part is then to finally formally introduce ourself to tensor product and it's importance for composite quantum systems.

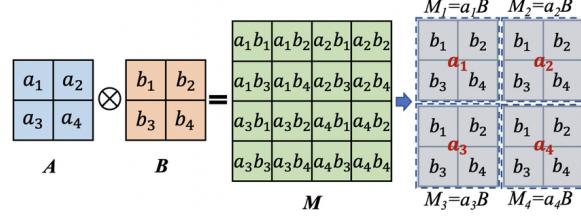


Figure 3.1: Matricial Representation of Tensor Product [35]

#### 3.1 Definition and Properties of Tensors

“Tensors are a generalization of vectors and matrices. A  $d$ -dimensional vector can be considered an element of  $\mathbb{C}^d$ , and a  $n \times m$ -dimensional matrix an element of  $\mathbb{C}^{n \times m}$ . Correspondingly a rank- $r$  tensor of dimensions  $\prod_{i=1}^r d_i$  is an element of  $\mathbb{C}^{d_1 \times \dots \times d_r}$ .

We can see that scalars, vectors and matrices are all rank 0, 1 and 2 tensors respectively.”

—Jacob C. Bridgeman, Christopher T. Chubb (2016)

Let  $V$  be a vector space of finite dimension  $n$ , and its dual base  $V^* = \{f : V \rightarrow \mathbb{K} \mid f \text{ linear}\}$ . Moreover, let  $r, s \in \mathbb{R}$ , then  $V^s = \prod^s V$  and  $(V^*)^r = \prod^r V^*$  [6].

**Definition 3.1.1** We call **Tensor of type**  $(r, s)$  on  $V$ , the bilinear map such that :

$$T : (V^*)^r \times V^s \rightarrow \mathbb{K} \text{ (usually } \mathbb{C}) \quad (3.1.1)$$

The set of all tensors of type  $(r, s)$  over  $V$  is denoted by  $\mathcal{T}_s^r(V)$

**Properties 3.1.2** The set  $\mathcal{T}_s^r(V)$  possesses fundamental properties:

1. Let  $V \subset \mathbb{K}$ , then  $\mathcal{T}_s^r(V)$  is also a vector space over  $\mathbb{K}$ . this implies that  $\forall T, T' \in \mathcal{T}_s^r(V), \forall \lambda \in \mathbb{K}$  :

$$(T + \lambda T')(\phi_1 \rightarrow \phi_r, v_1 \rightarrow v_s) = T(\phi_1 \rightarrow \phi_r, v_1 \rightarrow v_s) + \lambda T'(\phi_1 \rightarrow \phi_r, v_1 \rightarrow v_s) \quad (3.1.2)$$

Where  $\phi_i \in V^*$  and  $v_j \in V$

2. Let  $\dim(V) = n$ , then,  $\dim(\mathcal{T}_s^r(V)) = n^{r+s}$
3. The definition of tensors is basis-independent and doesn't rely of the choosed basis for  $V$ .

### 3.2 Tensors Product

**Definition 3.2.1[15]** Let  $V$  and  $W$  be two vector spaces over  $\mathbb{K}$ , then, we call **tensors product** of  $V, W$  the vector space  $V \otimes W$  and introduce the bilinear symmetric application  $\phi$  such that :

$$\begin{aligned}\phi : E \times F &\rightarrow E \otimes F \\ (x, y) &\mapsto x \otimes y\end{aligned}\tag{3.2.1}$$

Following the **universal property** defined as :

$\forall G \subset \mathbb{K}, \forall g$  of  $V \times W \rightarrow G$  bilinear map, then, there exists a unique linear map  $\tilde{g}$  of  $V \otimes W \subset G$  such that,

$$g = \tilde{g} \circ \phi \iff \forall x \in V, y \in F; g(x, y) = \tilde{g}(x \otimes y)\tag{3.2.2}$$

This property implies that  $(V \otimes W, \phi)$  is unique up to isomorphism.

**Properties 3.2.2** The Tensor Product is also ruled by the following properties :

1. Associativity :

Let  $U, V, W$  be vector spaces over  $\mathbb{K}$ , then :

$$(U \otimes V) \otimes W = U \otimes (V \otimes W)\tag{3.2.3}$$

2. Commutativity :

Let  $V, W$  be vector spaces over  $\mathbb{K}$ , then :

$$V \otimes W = W \otimes V\tag{3.2.4}$$

3. Dimension :

Let  $\dim(V) = n$  and  $\dim(W) = m$ , then :

$$\dim(V \otimes W) = mn\tag{3.2.5}$$

4. Distributivity :

Let  $U, V, W$  be vector spaces over  $\mathbb{K}$ , then :

$$(U + V) \otimes W = U \otimes W + V \otimes W\tag{3.2.6}$$

5. Duality :

Let  $V, W$  be vector spaces over  $\mathbb{K}$ , then :

$$(V \otimes W)^* = V^* \otimes W^*\tag{3.2.7}$$

**Example 3.2.3 — Tensor product  $\mathbb{C}^2 \otimes \mathbb{C}^2$**  Let  $V, W$  be two vector spaces of  $\mathbb{C}^2$ , let  $\{e_0, e_1\}$  and  $\{e'_0, e'_1\}$  be bases of respectively  $V$  and  $W$ , then,

$$\{e_0 \otimes e'_0, e_0 \otimes e'_1, e_1 \otimes e'_0, e_1 \otimes e'_1\} \text{ is a basis of } \mathbb{C}^2 \otimes \mathbb{C}^2 = \bigotimes_{i=1}^2 \mathbb{C}^2\tag{3.2.8}$$

This space is crucial in quantum computing systems, as it allows us to represent the state of two qubits and can be expanded for a  $n$ -qubits system using  $\bigotimes_{i=1}^n \mathbb{C}^2$ . For example, the maximally intricate state for a 2 qubits system — Bell State — can be written as  $\frac{1}{\sqrt{2}}(e_0 \otimes e'_0 + e_1 \otimes e'_1)$ .

### 3.3 Tensor Product of Linear Operators

**Definition 3.3.1** [28] Let  $E, F$  be vector spaces over  $\mathbb{K}$ , and let  $\mathcal{L}(E), \mathcal{L}(F)$  be the set of linear endomorphisms of respectively  $E, F$ .

Then, for any  $A \in \mathcal{L}(E), B \in \mathcal{L}(F)$ , we call **tensor product operator**  $A \otimes B \in \mathcal{L}(E \otimes F)$  the unique linear map such that :

$$(A \otimes B)(x \otimes y) = (Ax) \otimes (By), \quad (3.3.1)$$

and extended by linearity to all of  $E \otimes F$ .

#### Properties 3.3.2

1. Multiplication :

$$(A_1 \otimes B_1)(A_2 \otimes B_2) = (A_1 A_2) \otimes (B_1 B_2) \quad (3.3.2)$$

2. Trace Factorization :

Let  $E, F$  be two finite-dimentional vector space over  $\mathbb{K}$ ,

$$\text{Tr}(A \otimes B) = \text{Tr}(A) \text{Tr}(B) \quad (3.3.3)$$

3. Operator Norm :

Let  $E, F$  be Hilbert Spaces and  $A, B$  bounded, then :

$$\|A \otimes B\| = \|A\| \|B\| \quad (3.3.4)$$

4. Structure :

On all operations, the tensor product of the left factor inherits the algebraic structure from the right factor.

#### Example 3.3.3 — 2 dimensional Pauli gates [28]

Let  $X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$  be two one-dimensional — 1 qubit — Pauli gates. Using what we've seen above, their tensor product is :

$$X \otimes Z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad (3.3.5)$$

This product is now a two-dimensional gate operating a  $X$  transform on the first qubit, and a  $Z$  transform on the second one, this implies that for  $a, b$  two qubits of a system  $|\psi\rangle$  :

$$(X \otimes Z)|ab\rangle = |1-a\rangle \otimes (-1)^b|b\rangle, \text{ with } a, b \in \{0, 1\}. \quad (3.3.6)$$

**Remark 3.3.4** This example allows us to better understand how multi-qubit gates and complex circuits can be created from single-qubit gates, only using their tensor products. We will dive in-depth into complex gates and their properties in [part 3.1.1](#).

### 3.4 Quantum Applications

**Property 3.4.1** Let  $|\psi\rangle$  be a quantum state, then  $|\psi\rangle$  is separable (i.e., not entangled) if and only if :

$$\exists (|\psi_1\rangle, |\psi_2\rangle) \in \mathcal{H}^2 : |\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \quad (3.4.1)$$

**Remark 3.4.2 — Application** This idea is more than useful when conceiving algorithms centered about superposition, as it can't provide a simple test to determine if a state is entangled or not. An example of such algorithms can be found in [part 4.3 to 4.4 of Chapter III](#) about BB84 and E91 cryptography.

**Property 3.4.3** Let  $\rho(\alpha)$  and  $\rho(\beta)$  be the two density matrices representing respectively system  $\alpha$  and  $\beta$ . Then the density matrix of the global system  $\alpha\beta$  is defined by :

$$\rho(\alpha\beta) = \rho(\alpha) \otimes \rho(\beta) \quad (3.4.2)$$

**Remark 3.4.4 — Application** This property is necessary when considering multiple quantum channels, such as in communication, or when modeling noises — who randomly act as either a constructive or destructive channel —

**Reminder 3.4.5** We can remind the main property seen before using this example :



Figure 3.2: Visual Representation of a Bipartite Entangled State

The black and orange regions represent locally pure basis states  $|\psi_A\rangle$  and  $|\psi_B\rangle$ , while the in-between area corresponds to a non-factorizable component of the global state, e.g.,  $|\phi\rangle = \alpha|0\rangle_A|1\rangle_B + \beta|1\rangle_A|0\rangle_B$ .

The cat delimits the total system, whose reduced density matrices  $\rho_A = \text{Tr}_B(|\psi\rangle\langle\psi|)$  and  $\rho_B = \text{Tr}_A(|\psi\rangle\langle\psi|)$  are mixed, reflecting the entangled nature of the state.

## 4 Observables, Operators, Projectors

### 4.1 Observables & Operators

**Definition 4.1.1 — Operator** [28] Let  $\mathcal{H}$  be a Hilbert Space, then, we call **operator**  $A$  on  $\mathcal{H}$  the linear map  $A : \mathcal{H} \rightarrow \mathcal{H}$  such that if  $C \in \mathbb{R}, C \geq 0$ :

$$\|A\psi\| \leq C\|\psi\|, \forall \psi \in \mathcal{H} \quad (4.1.1)$$

The **operator norm** of  $A$  is then defined by :

$$\|A\| = \inf \left\{ C \geq 0 : \|A\psi\| \leq C\|\psi\| \forall \psi \in \mathcal{H} \right\} = \sup_{\|\psi\|=1} \|A\psi\| \quad (4.1.2)$$

Operators are the main brick of transformations inside a Hilbert space, by encapsulating any specific evolution that a state might face.

**Definition 4.1.2 — Observable** In quantum mechanics, we call **observable**, a Hermitian (i.e.  $A = A^\dagger$ ) operator  $\hat{O}$  acting on a Hilbert space  $\mathcal{H}$ .

The possible outcomes of measuring  $\hat{O}$  on a state  $|\psi\rangle$  are its real eigenvalues  $\lambda_i$ , and the post-measurement state is projected onto the corresponding eigen-space — following the entropy principle and application of its **projector**—.

**Properties 4.1.3** Let  $\hat{O}$  be an observable of  $|\psi\rangle$  on  $\mathcal{H}$ , then we can apply the following assertions :

1. Hermiticity :

$$\hat{O} = \hat{O}^\dagger \implies \lambda_i \in \mathbb{R} \quad (4.1.3)$$

2. Expectation value :

Let  $\hat{O} = \sum_i \lambda_i \Pi_i$ , then :

$$\langle \hat{O} \rangle_\psi = \langle \psi | \hat{O} | \psi \rangle = \sum_{i=0} \lambda_i \|\Pi_i |\psi\rangle\|^2 \quad (4.1.4)$$

### 4.2 Projectors

**Definition 4.2.1** We call **projector**  $\Pi$  on  $\mathcal{H}$  a Hermitian operator such that  $\Pi^2 = \Pi$ , Moreover,  $\sum_i \Pi_i = I \iff \Pi = \{\Pi_1 \rightarrow \Pi_n\}$  is a complete set of orthogonal projectors.

Operators allow us to formalize quantum state collapse, by projecting any vector onto a closed subspace  $V \subset \mathcal{H}$ , it isolates a subspace associated with a specific measurement result.

**Example 4.2.2** Let the Pauli  $Z$  operator defined by  $Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$  has eigenvalues  $\pm 1$ , with projectors  $P_{i+} = |0\rangle\langle 0|$ ,  $\Pi_- = |1\rangle\langle 1|$ . Measuring  $Z$  on  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  yields  $1$  with probability  $|\alpha|^2$ , and  $-1$  with probability  $|\beta|^2$ .

### 4.3 Concrete Quantum Application

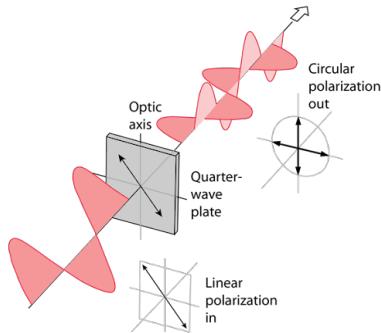


Figure 4.1: 45° Quarter-Wave plate's impact on a laser[19]

**Case Choosen 4.3.1 — Laser Polarization** A laser beam's polarization can be described using a  $2 \times 2$  matrix on  $|\psi\rangle = \alpha|H\rangle + \beta|V\rangle$  where  $|H\rangle$  denotes the horizontal basis and  $|V\rangle$  is the vertical basis.

The quarter-wave plate angled at degree  $\theta$  is the **unitary operator of the system**, we define the polarization of the beam as :

$$Q(\theta) = R(-\theta) \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} R(\theta), \quad (4.3.1)$$

Where  $R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$  is the matrix that rotates from angle 0 to angle  $\theta$ .

#### 4.4 Analysis of the case

In this example, the operators, projector, and observable are :

Type	Operator(s)	Projector	Observable
<b>Mathematical form</b>	$R(\theta), R(-\theta), Q(\theta)$	$\Pi(\phi) =  \phi\rangle\langle\phi $	$\{\Pi(\phi), I - \Pi(\phi)\}$
<b>Physical meaning</b>	Quarter-wave plate	polarizer at angle $\phi$	2 outcomes of the measure



### III Application to Quantum Computers

*“Analogous to the way a classical computer is built from an electrical circuit containing wires and logic gates, a quantum computer is built from a quantum circuit containing wires and elementary quantum gates to carry around and manipulate the quantum information.”*

— Nielsen, Michael A.; Chuang, Isaac (2010).

Hence, the objective of this chapter is to provide a comprehensive overview of quantum computing systems and their properties, using the algebraic definitions seen in chapter II.

#### 1 From Quantum States to Quantum Computers

Traditional computers use electric signals representing binary 1s and 0s (bits); a logical gate will take one or more bits for input and output the result of an operation assigned to it, permitting the running of any possible algorithm. Similarly, quantum gates are the fundamental operations that take as an input qubits and perform quantum calculations on them. There are several types of quantum gates divided into two categories: single-qubit gates and multi-qubit gates [2].

##### 1.1 Quantum Gates and Operations

**Definition 1.1.1 — Pauli Gates** The Pauli gates are single-qubit gates. We can note that they are involutory, meaning the square of a Pauli matrix is the identity matrix, i.e.  $I = X^2 = Y^2 = Z^2 = -iXYZ$ .

- **X gate :**

The X gate is the quantum version of the traditional NOT gate, it flips the state of the qubit, mapping  $|0\rangle$  to  $|1\rangle$  and  $|1\rangle$  to  $|0\rangle$  respectively. Its representative matrix is :

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (1.1.1)$$

- **Z gate :**

The Z gate introduces what's known as a **phase shift**,  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto -|1\rangle$  using the matrix :

$$Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.1.2)$$

- **Y gate :**

The Y gate acts as a combination of X and Z gates, acting both to creates a phase shift and flips the state of the qubit such that  $|0\rangle \mapsto i|1\rangle$  and  $|1\rangle \mapsto -i|0\rangle$ . We can represent Y as a matrix such that :

$$Y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (1.1.3)$$

**Definition 1.1.2 — Controlled gates** Let  $U$  be a single-qubit matrix given by  $U := \begin{pmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{pmatrix}$  (one of Pauli's matrices or the Hadamard gate for example),  
Then, the **Controlled- $U$  gate**  $CU$  is a 2-qubit gate defined by :

$$\begin{cases} |00\rangle \mapsto |00\rangle \\ |01\rangle \mapsto |01\rangle \\ |10\rangle \mapsto |1\rangle \otimes U|0\rangle = |1\rangle \otimes (u_{00}|0\rangle + u_{10}|1\rangle) \\ |11\rangle \mapsto |1\rangle \otimes U|1\rangle = |1\rangle \otimes (u_{01}|0\rangle + u_{11}|1\rangle) \end{cases} \quad (1.1.4)$$

Therefore, we can write the matrix of  $CU$  such that :

$$CU := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{pmatrix} \quad (1.1.5)$$

**Example 1.1.3** For example, in the case of the  $CX$  matrix (Controlled NOT), the gate performs the NOT operation on the second qubit, if and only if the first qubit is  $|1\rangle$ , its matrix is then :

$$CX := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (1.1.6)$$

**Definition 1.1.4 — Toffoli gate** Analogously to the Controlled NOT (CNOT) gate, a **Toffoli gate** is a 3-qubit CCNOT gate, the most common example of controlled-controlled-unitary gates, that performs an operation on the third qubit, if and only if the first two, the control qubits, are  $|1\rangle$ . Here, the operation is the Pauli matrix.

We can express it with the logical operators AND and XOR, for a 3-qubit input  $(a, b, c)$ , the output is  $(a, b, c \oplus (a \wedge b))$  and the representative matrix of the Toffoli gate is the following :

$$CCX := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (1.1.7)$$

**Remark 1.1.5** This gate is widely used for quantum error correction codes.

**Definition 1.1.6 — Phase shift/Rotation gate** This gate adds a relative phase shift of  $\theta$ , or rotates by  $\theta$  a qubit around a specific axis  $X, Y, Z$  :

$$R_X := \begin{pmatrix} \cos(\frac{\theta}{2}) & -i \sin(\frac{\theta}{2}) \\ -i \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{pmatrix} \quad (1.1.8)$$

$$R_Y := \begin{pmatrix} \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{pmatrix} \quad (1.1.9)$$

$$R_Z := \begin{pmatrix} \exp(-i\frac{\theta}{2}) & 0 \\ 0 & \exp(i\frac{\theta}{2}) \end{pmatrix} \quad (1.1.10)$$

**Definition 1.1.7 — Hadamard gate** The Hadamard gate, named after the French mathematician Jacques Hadamard, is perhaps the most important one.

It acts on a single qubit and it is the gate that creates the state of superposition (which is the main and most powerful characteristic of quantum computers) where a qubit simultaneously exists in both  $|0\rangle$  and  $|1\rangle$  with equal probability. It is essential for quantum parallelism, which refers to the possibility of executing multiple tasks at the same time, using quantum entanglement and superposition. The Hadamard gate is defined by :

$$\begin{cases} |00\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}} & \text{referred to as } |+\rangle \\ |01\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}} & \text{referred to as } |-\rangle \end{cases} \quad (1.1.11)$$

And can be represented by the matrix :

$$H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (1.1.12)$$

**Remark 1.1.8** Eventuellement elaborer sur la rotation sur la bloch sphere + hermitian hadamard

**Definition 1.1.9 — Swap Gate** The swap gate is self-explanatory, it swaps two qubits. The matrix for the swap gate is :

$$SWAP := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (1.1.13)$$

## 1.2 Register and Initialization

**Definition 1.2.1 — Quantum Register** A quantum register is a sequence of qubits. Unlike classical registers in a processor, quantum registers use superposition and entanglement to represent multiple states at once. A 2-qubit register can, for example, contain the four states  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$  and  $|11\rangle$  simultaneously.

Quantum registers are usually implemented using either superconducting circuits with artificial atoms as qubits, trapped ions or photons. In the very currently developing case of using photons, the process of producing a photon typically produces it in a fixed polarization which is measurable and alterable through a polarization filter if the basis state is not the one needed for computations. See image 1.1 below.

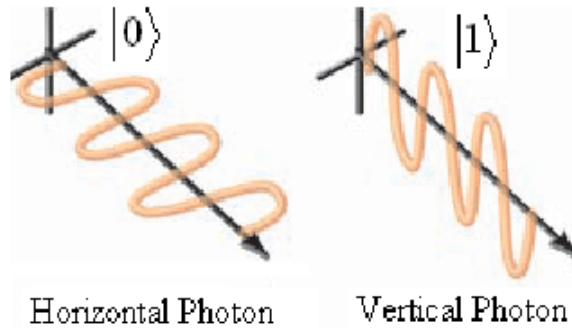


Figure 1.1: Encoding of a qubit in the polarization of a single photon[21]

Photons are widely used to represent qubits as they are very well isolated from their environment; their propagation through free space is comparable to a propagation through vacuum. This is in contrast to almost all other physical systems that exhibit quantum characteristics; they are subject to numerous disturbances from their environment.

For example, the spin of an electron can be used to encode a qubit, but it would be subject to noise due to interactions with anything that is charged or has a spin in its environment.

### Example 1.2.2 Example of initialization

### 1.3 Measurement and Collapse

**Definition 1.3.1** Quantum systems exist in superpositions of states, represented by a wavefunction, which means that a quantum entity, such as a qubit, can exist with probabilities of being in multiple states simultaneously, until it is observed.

The quantum measurement problem refers to this relationship between quantum systems and the act of measuring them. Quantum measurements actively influence the state of a qubit, forcing it into one definitive state, either  $|0\rangle$  or  $|1\rangle$ , based on inherent probabilities [29].

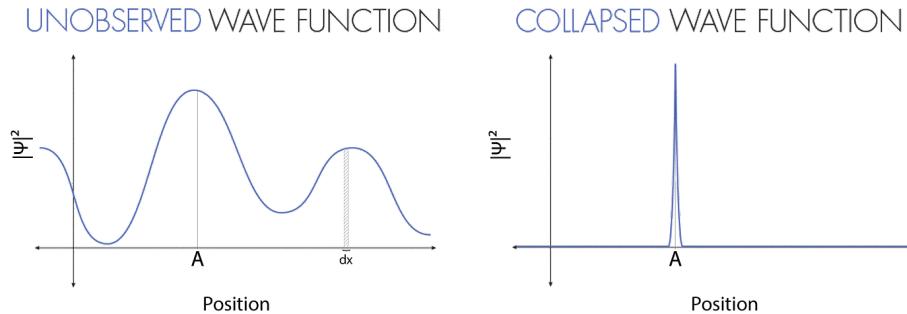


Figure 1.2: Collapse of the wave function upon observation[31]

**Remark 1.3.2** A measurement of a single qubit in a system of multiple qubits (a register) can affect and disturb the entire quantum system as well as induce errors but it is an indispensable process in quantum computing as it is how the results of computations are obtained.

**Remark 1.3.3** Measurements are irreversible, once the measurements are done, the original undisturbed system of superposed states can not be recovered.

**Remark 1.3.4** While there are probabilities concerning the pattern of a wave function collapse, it can not be predicted with certainty. This unpredictability is very valued in cryptography as random numbers are useful only if they are truly unpredictable.

### 1.4 From Logical Gates to Quantum Circuits

In the first section of this chapter, the main types of quantum logical gates have been detailed. When wiring these gates together we can create quantum circuits which we will detail in the next section. In section 1.2 has been explained the functioning of photonic quantum computers. In that case, the components of quantum circuits are implemented, among others, in the form of photodetectors, interferometers and beam splitters as photons they can not be held in place, so they are constantly moving through circuits at the speed of light and interacting with optical components.

In the case of trapped-ions quantum computers, qubits are represented using ions, or charged particles in a stable electronic state. Each ion can store a single qubit, which is encoded in the spin of the particle. They are confined in free space using electromagnetic fields, in order to preserve the fragile information.

To implement quantum gates in this case, there are a few different methods. For single-qubit gates, using a short pulse of microwave radiation, if the frequency of the microwave exactly matches the resonant frequency of the qubit, it will cause the qubit state to flip. It is also possible to create superposition states in the same way by adjusting how long the pulse lasts.

For multiple-qubit gates, the spin states used to store the qubits don't naturally interact with one another. The ions themselves do interact, however — they repel each other due to both having a positive electric charge, in a similar way to the repulsion between two bar magnets with their north poles facing each other.

Using this repulsion, lasers can be applied to induce an artificial interaction between the qubits. Lasers work for single-qubit gates as well to create an interaction between the qubit states.

**Remark 1.4.1** Provided two gates  $A$  and  $B$  both acting on the same number of qubits, if  $B$  is placed after  $A$  in a series circuit, the final result of these two gates combined can be expressed as a single new gate  $C$ , defined by :  $C = B \cdot A$  where  $\cdot$  is the matrix multiplication. Additionally,  $\dim(C) = \dim(A) = \dim(B)$ .

## 2 Quantum circuits

In computer science, circuits are models of computation in which information is carried by wires through a network of gates, which represent operations on the information carried by the wires. Quantum circuits are a specific model of computation based on this more general concept.

### 2.1 Principle and Particularity

**Definition 2.1.1** A **quantum circuit** is a model for a quantum computation. A computation is implemented in the form of quantum gates and measurements, using registers and qubits initialized to the needed values.

**Properties 2.1.2** Quantum circuits differ fundamentally from their classical counterparts in three main ways :

1. **Representation** : Every quantum gate must be represented by a unitary — hence reversible — operator  $U$  on the Hilbert space of the qubits. There is no analogue of an irreversible AND or OR gate. As such, information cannot be duplicated (no-cloning theorem).
2. **Destruction of Superposition** : Measurement in a quantum circuit is always destructive: when measuring a qubit, its superposition collapses to one outcome and the post-measurement state becomes a classical register as we seen in last part with gates. This measurement gate **cannot be undone** by subsequent unitary operations.
3. **Error Propagation** : the interplay of coherence and interference means that the global effect of a sequence of gates cannot be decomposed into independent subcircuits in the same way as for classical logic. This implies that tiny phase errors or unwanted entanglement can propagate nonlocally through the network

**Definition 2.1.3 — Complexity and circuit metrics** The resource cost of a quantum circuit is quantified by three primary metrics :

1. **The Circuit Width**  $n$  is the total number of qubits required.
2. **The Circuit Depth**  $d$  is the minimum number of sequential layers of gates that cannot be executed in parallel, reflecting the total coherence time needed.
3. **The Gate Count**  $G$  is the sum of all elementary gates used.

Optimizing these metrics under hardware connectivity and coherence constraints is central to making large-scale quantum algorithms practical.

## 2.2 Visual Representation

For easier communication in between engineers and comprehensibility of quantum circuits, a standardized visual representation for every gate that we have seen before has been implemented:

X gate	Y gate	Z gate	Hadamard gate	Controlled-Hadamard gate	CX gate	Swap gate	Rotation gates (example with Rx)	Toffoli gate

Figure 2.1: Representation of the main types of gates

In a quantum circuit, time flows from left to right. Quantum gates are ordered in chronological order with the left-most gate as the gate first applied to the qubits.

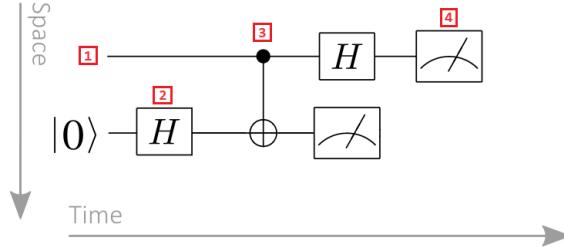


Figure 2.2: A Simplified Quantum Circuit [26]

Here, we have the following numbered component common to every quantum circuits:

1. **Qubit register:** Qubit registers are displayed as horizontal lines, with each line representing a qubit. The top line is qubit register labeled 0, the second line is qubit register labeled 1, and so on.
2. **Quantum gate:** Quantum operations are represented by quantum gates. The term quantum gate is analogous to classical logic gates. Gates acting on one or more qubit registers are denoted as a box. In this example, the symbol represents a Hadamard operation.
3. **Controlled gate:** Controlled gates act on two or more qubits. In this example, the symbol represent a CX gate. The black circle represents the control qubit, and the cross within a circle represents the target qubit.
4. **Measurement operation:** The meter symbol represents a measurement operation. The measurement operation takes a qubit register as input and outputs classical information.

### 2.3 Advanced Circuits

In the former section, we shown an example of a very simple quantum circuit to illustrate the definitions given, but quantum computers can be used to solve complicated problems. In this section, we will be explaining two famous algorithms, the Deutsch-Jozsa algorithm and the Schor algorithm.[9]

**Algorithm 2.3.1** The Deutsch-Jozsa algorithm is one of the first examples of a quantum algorithm that is exponentially faster than any possible deterministic classical algorithm.

The aim of the algorithm is to determine if a boolean function is balanced or constant. We take  $f$  to be a function that takes  $n$ -bit binary values as input and produces either a 0 or a 1 as output:

$$f : \{0, 1\}^n \longrightarrow \{0, 1\} \quad (2.3.1)$$

The function is said to be *balanced* if exactly half of the outputs are 0 and the other half are 1. It is said to be *constant* if all the inputs evaluate to either 0 or 1 exclusively.

Therefore, in the case of a one bit to one bit function, it is balanced if  $f(0) \neq f(1)$  and constant if  $f(0) = f(1)$ , we can deduce the following :

$$f(0) \oplus f(1) = \begin{cases} 0 & \text{if constant} \\ 1 & \text{if balanced} \end{cases} \quad (2.3.2)$$

From which we get the circuit :

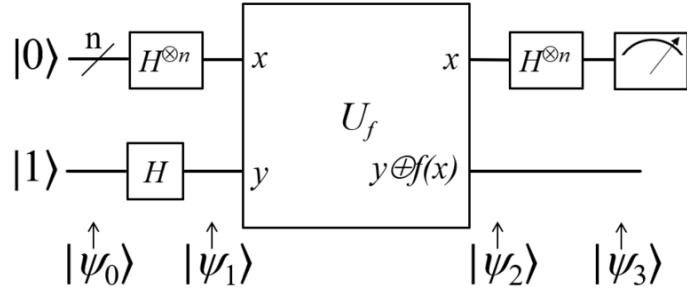
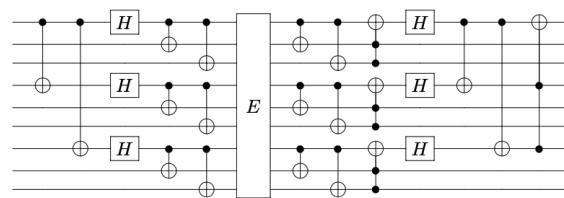


Figure 2.3: Quantum circuit associated to the Deutsch algorithm [30]

For a conventional deterministic algorithm where  $n$  is the number of bits,  $2^{n-1} + 1$  evaluations of  $f$  will be required in the worst case.











#### 4.4 Algorithms Comparison

Feature	BB84	E91
Type	Prepare-and-measure	Entanglement-based
Quantum object used	Single-photon (non-orthogonal) states $\{ 0\rangle,  1\rangle,  +\rangle,  -\rangle\}$	Maximally entangled pairs (Bell states) $\frac{1}{\sqrt{2}}( 00\rangle +  11\rangle)$
Encoding bases	Two mutually unbiased bases (Z, X) chosen at random	Local measurement in two conjugate bases; correlation tested via Bell bases/CHSH settings
Security principle	No-cloning theorem + QBER threshold (11% for intercept-resend attack)	Violation of Bell's (CHSH) inequality certifies security, even with untrusted source (device-independent)
Eavesdropping test	Compare subsets of raw key to estimate QBER	Estimate Bell parameter $S$ ; require $S > 2$ to bound eavesdropper's information
Key rate efficiency	$\approx 50\%$ of transmitted bits survive sifting	$\approx 50\%$ , plus Bell-test overhead
Implementation complexity	Relatively simple: weak coherent pulses or true single-photon sources	Requires reliable entangled-photon source and distribution
Assumptions	Trusted preparation device; perfect measurements	Device-independent security possible — untrusted source tolerated if Bell violation observed —

Table 1: Comparative overview of BB84 and E91 protocols

## IV Case study and Simulations

In the last chapter, we talked extensively about different quantum hardware. Complementarily, in this chapter we will overview different quantum software and simulation tools in order to study a specific case. The final goal of this part is to better understand the specificity of working with quantum circuits when performing actual computations.

### 1 Quantum Softwares

#### 1.1 Overview of Existing Platforms

When discussing quantum software programming, 3 different main platforms can be considered : Qiskit by IBM, CIRQ by Google, and QuTiP — an Open Source alternative —.

Platform	Qiskit	Cirq	QuTiP
Developer	IBM Quantum	Google Quantum AI	QuTiP Project
Main Usage	Gates, Machines learning	NISQ Circuits Engineering	Decoherence Simulation
Hardware Execution	Yes - IBM Q Experience	Yes - Google Sycamore	No
Coding language	Python	Python	CPython
Noise model	Markov's Noise	Pauli's Noise	Lindblad's equation

Each of those platforms benefits from their own pros and cons; as such, the choice of a specific one might be made solely on intended use case and the user's affinity with each language.

#### 1.2 Installation and Environment

Another point to be taken into consideration is the environment of programming. As all three are Python Libraries, they can simply be imported to a standard IDE after being downloaded from their respective websites:

- **Qiskit:** Install with `pip install qiskit`. Connect to IBM Quantum backends using an API token.
- **Cirq:** Install with `pip install cirq`. Integrate with Google Quantum Engine via GCP credentials for Sycamore access.
- **QuTiP:** Install with `pip install qutip`. Local-only simulations, no cloud hardware.

The main difference in their environment is then the possibility — or not —, to be directly connected to an actual quantum computer in the cloud.

### 1.3 Quantum Programming Languages

QASM, Python, OpenQASM, Q#

### 1.4 Practical Examples

Below is a simplified example of preparing and simulating a 3-qubit GHZ state on each platform.

#### Qiskit

```

1 from qiskit import QuantumCircuit, Aer, execute
2 qc = QuantumCircuit(3,3)
3 qc.h(0)
4 qc.cx(0,1)
5 qc.cx(1,2)
6 qc.measure([0,1,2],[0,1,2])
7 sim = Aer.get_backend('qasm_simulator')
8 res = execute(qc, sim, shots=1024).result()
9 print(res.get_counts())

```

#### Cirq

```

1 import cirq
2 qubits = cirq.LineQubit.range(3)
3 circuit = cirq.Circuit([cirq.H(qubits[0]),cirq.CNOT(qubits[0],
    qubits[1]),cirq.CNOT(qubits[1], qubits[2]),cirq.measure(*qubits, key='m')])
4 simulator = cirq.Simulator()
5 result = simulator.run(circuit, repetitions=1024)
6 print(result)

```

#### QuTiP

```

1 from qutip import basis, tensor, hadamard_transform, cnot, ket2dm, measurement_statistics
2 psi0 = tensor([basis(2,0)]*3)
3 ghz = cnot(2,1) * (cnot(1,0) * (tensor([hadamard_transform(), identity(2), identity(2)]) *
    psi0))
4 rho = ket2dm(ghz)
5 projectors = [basis(8,i)*basis(8,i).dag() for i in (0,7)]
6 stats = measurement_statistics(rho, projectors)
7 print(stats)

```

As we can see, each platform uses their own object to represent quantum circuits and qubits, with Qiskit and Cirq using native Python objects, whereas QuTiP depends on its own import. Moreover, we can see that Qiskit and Cirq provide directly in their run functions a way to directly repeat a simulation  $n$  times, allowing for better measurements and analysis.

## 2 Quantum Circuits simulation

### 2.1 Simulation Tools Comparison

Comparer les perfs de Qiskit, Cirq, QuTiP dans la simulation de circuits

### 2.2 Building and Running Circuits

Each simulation follows three steps:

1. **Circuit definition** in Python using the framework's API,
2. **Compilation** to the simulator's native format,
3. **Execution** and retrieval of outcomes (counts, state vectors, or density matrices).

Examples were provided in the previous section.

### 2.3 Measurement and Interpretation

Each Simulators return different data types:

- **Counts** (QASM) in Qiskit, for frequency histograms, with different data about the measurements made and stress on the system,
- **Measurement samples** via Cirq's `result.measurements`,
- **Density matrices** in QuTiP, from which probabilities and entropies are extracted.

Interpretation relies on statistical analysis of measurement results and comparison with theoretical predictions.





## 4 Case Studies

In order to conduct basic testing about the behavior of quantum circuits and algorithms, we chose to use IBM Fake\_provider's GenericBackendV2. In contrast, to evaluate real-world execution times and practical applications, we will rely on IBM's Actual Quantum Computers by using the classical Qiskit library.

For the simulations presented in this thesis, we interfaced with the state-of-the-art IBM Kyiv Quantum Computer, which is characterized by the following architecture :

Device Specifications	
Qubits	127
Processor Type	Eagle r3
Version	1.20.22
CLOPS	30K
Basis Gates	ECR, ID, RZ, SX, X
Performance Metrics	
2-Qubit Error (Best)	$4.03 \times 10^{-3}$
2-Qubit Error (Layered)	$1.52 \times 10^{-2}$
Median ECR Error	$1.098 \times 10^{-2}$
Median SX Error	$2.780 \times 10^{-4}$
Median Readout Error	$1.099 \times 10^{-2}$
Median T1	285.96 $\mu$ s
Median T2	112.57 $\mu$ s

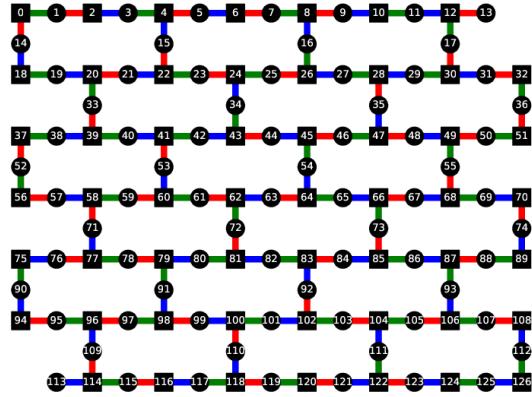


Figure 4.1: Table 1 and Figure 1.1: (Left) IBM Kyiv Quantum Processor Specifications and Performance[20] (Right) Heavy-hexagonal topology of 127-qubit IBM Eagle r3 processor.[39]

### 4.1 Deutsch-Jozsa Algorithm

The Deutsch-Jozsa Algorithm, developed in 1992 by two mathematicians : David Deutsch and Richard Jozsa [9].

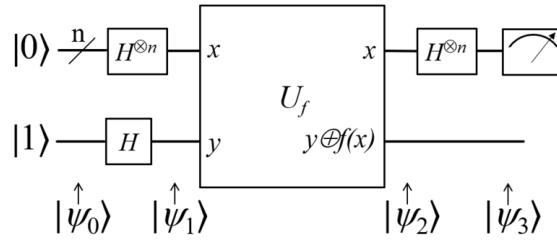


Figure 4.2: Deutsch-Jozsa Quantum Circuit[30]

For Qiskit's configuration and testing, we chose to use  $n$  qubits completed by an oracle qubit on top charged with verifying the others. This model allows us to observe the state of all qubits in one single operation. The code made for this can be found in Annex 1.

## 4.2 Hypothesis

1. the standard output for Constant function  $f$  is  $|\underbrace{0\dots0}_{n \text{ times}}\rangle$ .
2. On the other hand, the required output to be considered a Balanced function  $f$  is  $|\underbrace{0\dots0}_{n-1 \text{ times}} 1\rangle$

In each case, we will repeat our measures 1024 times in order to have a certain measurement independent of any noise that might affect our system.

## 4.3 Results Obtained

### 4.3.1 Quantum Circuits Generated

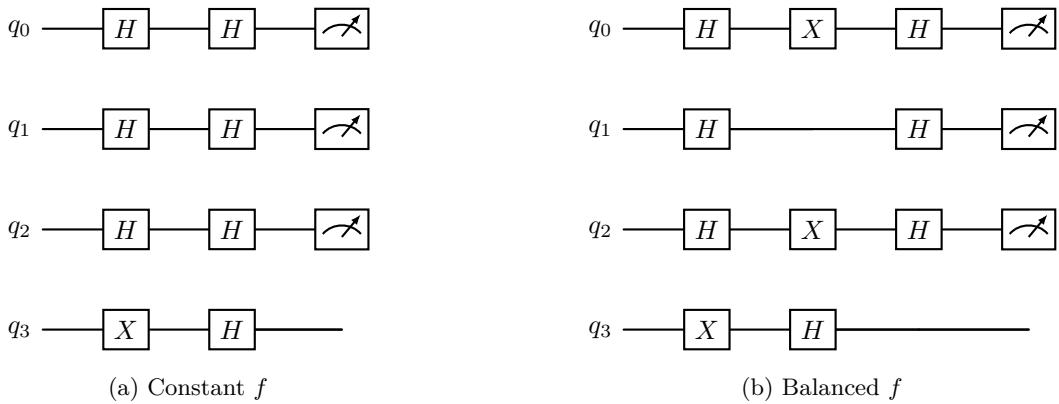


Figure 4.3: Comparison of Deutsch–Jozsa Qiskit's Quantum Circuits from [Annex 1](#)

### 4.3.2 Measurement outcomes

(a) Constant Oracle (a)		(b) Balanced Oracle (b)	
State	Frequency	State	Frequency
$ 100\rangle$	3/1024	$ 101\rangle$	1/1024
$ 010\rangle$	2/1024	$ 011\rangle$	2/1024
$ 000\rangle$	1019/1024	$ 000\rangle$	4/1024
		$ 001\rangle$	1017/1024

Table 2: Measurement outcomes from the Constant and Balanced Oracles

#### 4.4 Analysis and Discussion

As we can see, the measurements yield, for the vast majority of them, their anticipated results — $|000\rangle$  for the constant Oracle and  $|001\rangle$  for the balanced counter-part—. But more interesting is that we were able to measure a few in-between outcomes such as  $|100\rangle$ ,  $|101\rangle$ ,  $|011\rangle$ , etc. Those results, independent from errors in the code or the protocol, are actually the incarnation of what we discussed about the uncertainty proper to the quantum state.

More specifically, those parasitic measurements are the direct consequence of noise's impact on the system and the probabilistic nature of qubits, even if calculation should make our final state 100%  $|000\rangle$  or  $|001\rangle$ . In practice, noise tends to mix up our solutions turning it into :

$$\text{Oracle outcome} = \begin{cases} \{|000\rangle (a), |001\rangle (b)\} & : 99.414 \pm 0.0097\%, \\ \text{other} & : 0.586 \mp 0.098\%. \end{cases} \quad (4.4.1)$$

This implies that we managed to observe the properties discussed in this thesis for ourselves using this experiment, therefore confirming our predicates.

## V Conclusion

In this work, we have developed a unified algebraic framework for the characterization of mixed quantum states — tailored to the needs of quantum computing systems —.

We began by recalling the fundamental notions of Hilbert spaces, Dirac notation, pure versus mixed states and their statistical, algebraic and geometric representations — wave mechanics, matrix mechanics, density operators, Bloch sphere — .

We then introduced a family of spectral invariants—beyond the standard trace and purity—that are sensitive to decoherence and interference, and demonstrated their computation via operator-algebraic tools ( $C^*$ -algebras and Von Neumann-algebras, spectral decomposition, partial trace, etc).

In Chapter III, we showed how these mathematical objects can be translated into concrete quantum gates and circuits. We reviewed single-qubit and multi-qubit gates (Pauli, Hadamard, phase rotations, controlled and Toffoli gates), formalized their unitary matrices and tensor-product constructions, and discussed resource metrics — circuit width, depth, gate — . We also highlighted the distinctive features of quantum versus classical circuits — reversibility, no-cloning, measurement collapse and error propagation — and presented standard diagrammatic conventions.

Chapter IV was devoted to a case study and simulations. We compared simulator performances and models, and carried out the Deutsch–Jozsa algorithm both on IBM’s Aer simulator and on a real 127-qubit Eagle r3 device. The experimental results confirmed (i) the practical relevance of our spectral invariants to diagnose decoherence, and (ii) the theoretical predictions concerning balanced versus constant oracles, up to NISQ-level noise.

## Annexes

Annex 1: Local Version of Quantum Deutsch–Jozsa Algorithm using Qiskit

```
1 import time
2 from qiskit import QuantumCircuit, transpile
3 from qiskit.providers.fake_provider import GenericBackendV2
4 from IPython.display import display
5
6 def create_constant_oracle(n,out):
7     o=QuantumCircuit(n+1)
8     if out:o.x(n)
9     return o
10
11 def create_balanced_oracle(n):
12     o=QuantumCircuit(n+1);o.cx(0,n);return o
13
14 def dj_circuit(o,n):
15     c=QuantumCircuit(n+1,n);c.x(n)
16     for q in range(n+1): c.h(q)
17     c.compose(o,inplace=True)
18     for q in range(n):
19         c.h(q); c.measure(q,q)
20     return c
21
22 def run_test(n,oracle='constant',c_out=0):
23     s=time.time()
24     is_const=True;p=None
25     for x in range(2**n):
26         v=c_out if oracle=='constant' else((x>>(n-1))&1)
27         if p!=None and v!=p: is_const=False;break
28         p=v
29     t_classic=time.time()-s
30     print(f"Classical method: {t_classic:.6f} s, {n**2-1} Operations -> {'CONSTANT' if
31         is_const else 'BALANCED'}")
32     o=create_constant_oracle(n,c_out) if oracle=='constant' else create_balanced_oracle(n)
33     print(f"Using a {oracle.upper()} oracle.")
34     c=dj_circuit(o,n);display(c.draw())
35     backend=GenericBackendV2(num_qubits=5)
36     job=backend.run(transpile(c,backend),shots=1)
37     counts=job.result().get_counts()
38     r=max(counts,key=counts.get)
39     print("Outcomes:",counts)
40     print("Conclusion:", "CONSTANT" if r=='0'*n else "BALANCED")
41
42 run_test(3,'constant',0)
43 print("\n"+"*50+"\n")
44 run_test(3,'balanced')
```

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