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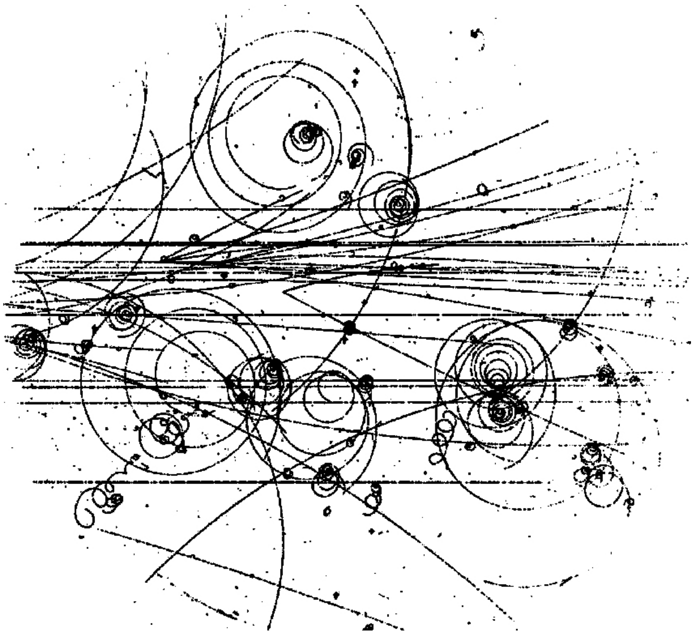
QUANTUM COMPUTING FOR LOGICAL INFERENCE

Subtitle



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Part I

THEORETICAL BASES

1 QUANTUM MECHANICS

In this chapter we will explore the basics of quantum mechanics in order to understand what we can or cannot do with a quantum computer. The reference architecture for this work is the quantum gate-based quantum computer. In the next pages we will try to justify why the algorithms that run on this hardware need to be reversible.

The chapter starts from the very beginning with the definition of a quantum system and presents the basis to understand the evolution of a quantum system, trying to justify why every evolution needs to be reversible and what exactly reversibility means. At the end of the chapter we will put all of our new knowledge together to derive the famous Schrödinger equation.

With all this work we will be able to imagine the function of a quantum gate and understand the limitations that are imposed when we develop an algorithm for a quantum computer.

1.1 EXPERIMENTS

We start our introduction to quantum mechanics with an experiment. Experiments are not only an excuse to introduce the topic, but the essential key of physics, both classical and modern.

Theory and models need to adapt to the experiments, and when the experimental results are in contradiction with the actual model it means that the model needs to be changed to respect the behavior of the world.

1.1.1 Spin

We analyze the experiment of an electron in a magnetic field. An electron is an electrically charged particle; when some electrons are shot in an electric field all of them are influenced by Coulomb's law; if all electrons have the same initial velocity the beam of electrons remains intact.

What happens to the same beam in a magnetic field? Again electrons are deflected by a force, but this time the beam splits. If the initial velocity was parallel to the x axis and the magnetic field is oriented along the z axis some electrons are deflected upward, some downward, but the intensity of the deflection is the same for all the electrons. This means that no electrons are deflected less or more than the others and the beam splits exactly into two parts.

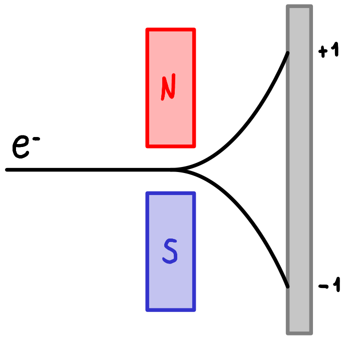

Figure 1.1: Experiment's schema

Starting from this experiment we can make a measuring instrument: this apparatus $\mathcal{A}$ can be oriented along an arbitrary axis, and in the previous configuration $\mathcal{A}$ displays $+1$ if the electron is deflected upward, -1 otherwise. We call this number the spin of the electron.

Repeatability of measure

If we measure the spin of an electron and $\mathcal{A}$ displays $+1$, we can confirm the experiment's results by measuring the spin again and we obtain spin $+1$ every time. This means that the measurements are repeatable (an essential property to construct models and make predictions). We can think, and it will be clear later why it is useful, that the first experiment prepares the spin $+1$ and the others confirm this result.

Spin is a quantum property and all the visual representations such as the rotation of the electron around its axis would lead to misrepresentation. Spin and rotation, however, have some similarities. Let's analyze what would happen if we consider a charged sphere in a magnetic field with the laws of classical physics. We consider a sphere rotating around its axis, and this axis is parallel to the z axis. The x or y component of the angular momentum is zero. Measuring the component along a generic axis, oriented like the versor $\hat{n}$[1], we would obtain a result proportional to the projection of $\hat{z}$ on $\hat{n}$. This projection can be found with the scalar product $\hat{z} \cdot \hat{n} = \cos\theta$[2], where θ is the angle between the axes.

Now we consider the quantum version of this phenomenon. Let's start by measuring the z component of the spin and assume that the result is $\sigma_z = +1$; if we rotate the apparatus $\mathcal{A}$ around, for example, the x axis, we can measure σ_x. This component would not be zero, and $\mathcal{A}$ keeps displaying only $+1$ or -1. The single result is not helpful, but we can repeat the experiment, namely:

1. orienting $\mathcal{A}$ along the z axis and preparing a spin $\sigma_z = +1$
2. rotating $\mathcal{A}$ around x
3. measuring the x component of the spin

statistically we would observe the same number of $\sigma_x = +1$ and $\sigma_x = -1$.

If we start the experiments with a spin prepared as $\sigma_z = +1$ and then orient $\mathcal{A}$ along a generic axis $\hat{n}$ each measure would be binary and unpredictable, but the mean of the measures tends to $\hat{z} \cdot \hat{n} = \cos\theta$ where θ is the angle between $\hat{z}$ and $\hat{n}$. In the most general case we can start with the apparatus oriented like m and prepare the spin $\sigma_m = +1$, then we rotate $\mathcal{A}$ around $\hat{n}$ without interfering with the spin and measure again; we would obtain the statistical result $\langle \sigma_n \rangle = \hat{m} \cdot \hat{n}$[3].

The result of a single measure is non deterministic, but we can make predictions over the mean values of the measures: the expected values behave as the single results of the classic experiment.

Invasive experiment

Considering now a sequence of three measures: starting with $\mathcal{A}$ oriented along z we prepare the spin $\sigma_z = +1$, then we rotate $\mathcal{A}$ to measure σ_x obtaining, let's say, $+1$ (the reasoning is the same if we obtain -1); lastly returning with $\mathcal{A}$ parallel to z we cannot make any prediction on the single result, the initial configuration (with $\sigma_z = +1$) is lost forever, the only result we can predict is that $\langle \sigma_z \rangle = 0$.

---

[1] A versor is a vector of magnitude 1 (unit vector), it is normally used to specify a direction.

[2] We can use directly the angle because we are considering versors.

[3] The Dirac bracket $\langle\ \rangle$ denotes the statistical mean of a quantity. We call that expectation value.

1.1.2 Qubit

We have introduced the spin referring to electrons in a magnetic field. However, we can study the spin without examining the associated electron; we have isolated a simple physical system, the simplest we can study.

Spin belongs to a class of simple physical systems called *qubit*; in all of these systems the result of a measure is binary. We will see that, even if the result of a measure is equal to the classical *bit*, the qubit system is described in a very different way compared to its classical alter ego.

1.1.3 Boolean Logic

In this paragraph we try to understand why we need two different ways to describe a classical and a quantum state space. To do so we analyze the results of some logical propositions, both basic and composed via logical connectives.

Starting with the classical case we consider a bag of colored and numbered balls. We can construct the state space by enumerating all states, namely taking each ball from the bag and annotating the pair number–color. The basic propositions we analyze are:

- The extracted ball is red.
- The number on the extracted ball is even.

If we consider a particular state we can say if a proposition is true or false; we can also define two subsets of balls, the first with all the red balls (for this subset the first proposition is true), the second one with the balls that show an even number (subset that makes the second proposition true). Considering now disjunction and conjunction:

- The extracted ball is red *or* even.
- The extracted ball is red *and* even.

Again it is simple to associate a truth value to these propositions if we consider a single state; also we can construct two subsets that satisfy the propositions from the subsets we defined before: the new subsets are respectively the union and intersection of the old ones.

In the quantum world the situation is very different. Let's start from propositions that can be verified with a simple experiment:

- The z component of the spin is $+1$.
- The x component of the spin is $+1$.

If we want to check the first proposition we can orient the apparatus $\mathcal{A}$ along z and make a measurement; the same procedure can be followed for the second proposition. The disjunction and conjunction of these propositions are:

- The z component of the spin is $+1$ *or* the x component is $+1$.
- The z component of the spin is $+1$ *and* the x component is $+1$.

The disjunction is not commutative

Starting with the disjunction. Considering a state prepared, without our knowledge, with $\sigma_z = +1$. If our first measure is along the z axis, $\mathcal{A}$ will always display $+1$ and we can immediately conclude that the proposition is true. If we start measuring the x component, we have a 50% chance that $\mathcal{A}$ displays $+1$ or -1; also this measurement destroys the initial state and the measure of σ_z becomes non predictable. In this scenario we have a 25% chance of deducing that the proposition is false; figure 1.2 shows all the possible measurement results in this case. The logical value of a proposition depends on the order in which we perform the measurements.

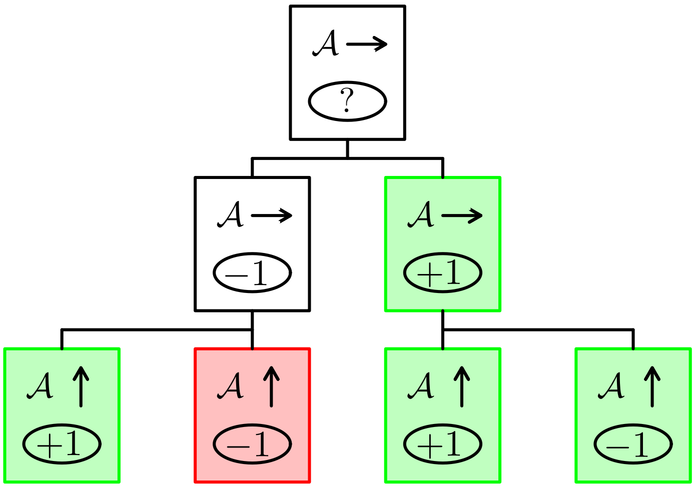

Figure 1.2: The apparatus $\mathcal{A}$ is represented as a box, the arrow represents the direction along which the apparatus is oriented, the display (ellipse) shows the result of measurement. We have highlighted in green the cases in witch we can immediately conclude that the disjunction of the propositions is true

The conjunction loses its meaning

The conjunction is even worse: no matter the order of the measurements, the second one destroys the result of the first. The disjunction is true if at least one of the sub-propositions is true, and if we find a spin component that is $+1$ we can always confirm this result with another measurement. In the conjunction the two sub-propositions must be true *at the same time*, but with the second measurement we lose all the knowledge of the first one. We can never conclude that the conjunction is true.

1.2 QUANTUM STATES

In the previous section we have understood that a state space of a quantum system cannot be represented in the same way as a classical state space. Now we present a formal mathematical model to describe the state space for spin.

Axiom 1. *The state space for a quantum system is a complex vector space.*

This is a physical axiom, which means that it is true because there are a lot of experiments that confirm this model and none that shows a contradiction.

1.2.1 Vector Spaces

A vector space is a mathematical and abstract construction that can have multiple dimensions (even infinite) and has, as components, integers, real or complex numbers, or other elements. An example that shows well how abstract a vector space can be is the complex-valued continuous function of variable x; the set of these functions generates a vector space.

Hilbert space

In quantum mechanics the state space is described by a vector space having as element $|A\rangle$ called *ket*. The properties of this space are:

- the sum of two kets is a ket;
- addition is commutative;
- addition is associative;
- existence of identity element for addition;
- existence of inverse elements for addition;
- existence of identity element for scalar multiplication;
- linearity property.

1.2.2 Bra and Ket

An example of ket that we will find often is the column vector of two dimensions:

$$|A\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

where α_1 and α_2 are complex numbers. With this simple example of ket it is easy to verify the validity of all previously described properties.

If, for complex numbers, exists the complex conjugate, for every ket there exists a *bra*. The set of bra generates a dual conjugate space with respect to the state space of ket. We denote a bra as $\langle A|$. If $|A\rangle$ is the ket of the previous example the corresponding bra is a row vector having as elements the complex conjugate of $|A\rangle$:

$$\langle A| = (\alpha_1^*, \alpha_2^*)\,.$$

Inner product

Name and symbol associated with elements of Hilbert spaces become clear when we define the product *bra-ket*, this is the corresponding scalar product of an ordinary vector and is called inner product. Considering bra and ket of two dimensions we can evaluate the inner product by adding the products of corresponding components:

$$\langle A\,|\,B\rangle = (\alpha_1^*, \alpha_2^*) \cdot \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = \alpha_1^*\beta_1 + \alpha_2^*\beta_2.$$

Having the inner product we can define:

VERSOR normalized vector $|A\rangle$ in which $\langle A\,|\,A\rangle = 1$;

ORTHOGONAL VECTOR vectors that have a null inner product: $\langle A\,|\,B\rangle = 0$.

We are familiar with these concepts in two and three dimensions, the first one is a vector of length one, the second is the right angle between two vectors. This representation is misleading in our case, we cannot imagine a ket like an arrow and the state space is completely abstract even if there are properties and operations in common between this space and the 3D space that we are familiar with.

We have lost the geometric interpretation, and it seems that we have defined two completely abstract and useless concepts, we will see next that these are key concepts in the description of quantum systems and have a precise and important physical meaning.

Orthonormal basis

By having a vector space is possible to build a set of orthogonal versors that generates all vectors in the given space. This set is called orthonormal basis and the cardinality of the set is equal to the dimension of the space.

Formally having a basis $\mathscr{B} = \{ |i_1\rangle, |i_2\rangle, \dots, |i_N\rangle \}$ of a space with N dimensions, we can write a generic vector in that space as

$$|A\rangle = \sum_{n=1}^{N} \alpha_n |i_n\rangle = \sum_{n=1}^{N} |i_n\rangle \langle i_n | A\rangle \tag{1.1}$$

this is the linear combination of the basis versors; where kets $|i_n\rangle$ are the versors in the basis and α_n are the vector components. We can obtain those components with the inner product between the vector $|A\rangle$ and the basis versors:

$$\alpha_i = \langle i | A\rangle . \tag{1.2}$$

1.2.3 Hidden variables

In a classical system we can measure all the variables associated to a physical system and then make a deterministic prediction of the evolution of that system. From the experiments described in the first section we have learned that a quantum system is not completely predictable even if we can make all the measurements that we want[4]. We can ask ourselves if our measurements aren't enough, if there are other variables that can make the prediction completely deterministic. About that topic we don't have any experimental proof, the opinion of physicists is divided in two main visions:

OPINION ONE : there are hidden variables and, if we manage to measure them, the prediction of results become deterministic. These variables can be

- very difficult to measure
- unknowable to us because also we are constituted by quantum material.

OPINION TWO : hidden variables don't exist, we already know all the information about a given system and quantum mechanics is intrinsically non deterministic.

No hidden variables

Probably no experiment could determine which vision is correct, but this doubt doesn't worsen our comprehension of the physical world. We can simply choose one vision and build our model coherently. We choose the simpler one, without hidden variables, all that we have to model are the quantities that we can measure and the measurements allow us to know all the information about a given system.

---

[4] We remember that a measure along one axis destroys our knowledge about the result along another axis.

Even if we have lost complete determinism, knowing the state of a system gives us some information about the system and the successive measurements. In the next section we will see what we can deduce about spin.

1.2.4 Spin states

Let's start enumerating all possible spin states along the coordinate axes. If we rotate the apparatus $\mathcal{A}$ around z, we can obtain $\sigma_z = \pm 1$; we call these states *up* and *down* and label them with kets $|u\rangle$ and $|d\rangle$. Orienting $\mathcal{A}$ along x, we obtain *left* $|l\rangle$ and *right* $|r\rangle$. Lastly, along the y axis, we measure the states *in* $|i\rangle$ and *out* $|o\rangle$.

Spin space states have two dimensions

The hypothesis that there aren't hidden variables allows us to represent the space state in a simple way: each spin state can be represented as a ket in a two-dimensional complex vector space.

To express a vector we need a basis; we choose $\mathscr{B} = \{\, |u\rangle, |d\rangle \,\}$[5] and try to obtain all states as a linear combination (*superposition*) of the basis vectors. A generic state $|A\rangle$ can be expressed as:

$$|A\rangle = \alpha_u |u\rangle + \alpha_d |d\rangle$$

where α_u and α_d are the components of $|A\rangle$ along $|u\rangle$ and $|d\rangle$, and can be obtained by projection: $\alpha_u = \langle u \,|\, A\rangle$ and $\alpha_d = \langle d \,|\, A\rangle$ (as in equation 1.2).

Probability amplitudes

$|A\rangle$ components are complex numbers and their physical meaning is: having a spin prepared in the state $|A\rangle = \alpha_u |u\rangle + \alpha_d |d\rangle$[6]; $\alpha_u^* \alpha_u$ is the probability of measuring $\sigma_z = +1$, while $\alpha_d^* \alpha_d$ is the probability that a measurement of σ_z will yield -1. Formally we can denote the probability of measuring $+1$ and -1 as P_u and P_d respectively and write:

$$\begin{aligned} P_u &= \langle A \,|\, u\rangle \langle u \,|\, A\rangle \\ P_d &= \langle A \,|\, d\rangle \langle d \,|\, A\rangle \,. \end{aligned} \tag{1.3}$$

Components α_u and α_d are called probability amplitudes, and their physical meaning is given by the square of the magnitude. This is the actual probability, and we want the sum of all probabilities to be one. This is equivalent to requiring that $|A\rangle$ is normalized: $\langle A \,|\, A\rangle = 1$.

Now we will show why $|u\rangle$ and $|d\rangle$ have to be orthogonal:

$$\begin{aligned} \langle u \,|\, d\rangle &= 0 \\ \langle d \,|\, u\rangle &= 0. \end{aligned}$$

We try to give an idea with a *reductio ad absurdum*: if $|u\rangle$ and $|d\rangle$ were not orthogonal, the projection of one on the other would not be null. This means that if we orient $\mathcal{A}$ along z and measure $\sigma_z = +1 = |u\rangle$, we would have $\alpha_d = \langle d \,|\, u\rangle \neq 0$, which is a contradiction to experimental results. If $\alpha_d \neq 0$, then $\alpha_d^* \alpha_d > 0$; we started with a state prepared as $\sigma_z = +1$ and ended with a nonzero probability of measuring $\sigma_z = -1$: this is absurd.

---

[5] We will show that these vectors are in fact orthogonal and why they need to be.

[6] From now on we use "prepared" or "measured" as synonyms: every measurement is invasive and can change the spin state, so no matter what was the previous state, after a measurement the state is the one we have measured.

Orthogonal states are mutually exclusive

We can extend the reasoning to a general and key concept of quantum mechanics: two orthogonal states are distinct and mutually exclusive. If the system is in the first state, the probability of finding it in the second is zero.

Now we are ready to express spin states as linear combinations of the basis vectors $\mathscr{B} = \{\,|u\rangle\,, |d\rangle\,\}$. The representation of the basis vectors themselves is naturally easy:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1.4}$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1.5}$$

To construct vector *right*, let's consider a spin prepared in the state $|r\rangle$. If we measure σ_z, we have a 50% chance of obtaining $+1$ (and 50% for -1); this means that for $|r\rangle$ we have $\alpha_u^* \alpha_u = \alpha_d^* \alpha_d = {}^1\!/_2$. A vector that satisfies this constraint is:

$$|r\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{1.6}$$

The reasoning is the same for state *left*; we also add the constraint that a state *left* cannot be *right* and vice versa: $\langle r \,|\, l\rangle = \langle l \,|\, r\rangle = 0$. We can express *left* as:

$$|l\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}. \tag{1.7}$$

Lastly, the constraints to find explicit forms for *in* and *out* are:

- states must be orthogonal: $\langle i \,|\, o\rangle = \langle o \,|\, i\rangle = 0$;
- if we have a spin prepared as *in* or *out*:
  - equiprobability of measuring $\sigma_z = +1$ and $\sigma_z = -1$;
  - equiprobability of measuring $\sigma_x = +1$ and $\sigma_x = -1$.

Two vectors that satisfy these constraints are:

$$|i\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} \tag{1.8}$$

$$|o\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix}. \tag{1.9}$$

This last derivation shows why it is important that the state space is complex: if we only accepted real components for our vectors, the system of equations we have implicitly defined would not have any solution[7].

---

[7] To avoid confusion, we point out that $|i\rangle$ is the ket of state *in*. i, instead, is the imaginary unit.

1.3 OBSERVABLES

We have learned that in classical mechanics we can trust our intuition, and we can do one or more measurements to know exactly the state of a system: a measurement does not perturb the state, which is the same before, during, and after the measurement.

In quantum mechanics the situation is more complex; our intuition is misleading, and we need mathematical tools to describe what we can measure: the observables. These tools are mathematical operators called *machines* (**M**) and have as both input and output state vectors.

Axiom 2. *Machines associated with observables are described by linear operators.*

We will show that machines are Hermitian operators, so let's start defining these operators and describing their properties[8].

1.3.1 Hermitian operator

Formally, machines modify a state vector in this way:

$$\mathbf{M}\,|A\rangle = |B\rangle$$

The linearity of machines implies that:

$$\mathbf{M}\,|A\rangle = |B\rangle \Rightarrow \mathbf{M}z\,|A\rangle = z\,|B\rangle$$

and:

$$\mathbf{M}(|A\rangle + |B\rangle) = \mathbf{M}\,|A\rangle + \mathbf{M}\,|B\rangle\,.$$

If we choose a basis to represent machines and state vectors, we can write explicitly the linear operator as an $N \times N$ matrix, where N is the dimension of the vector space of the state vectors. A generic machine that transforms spins can be expressed as:

$$\mathbf{M} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}.$$

When we fix a basis, we are forced to express all state vectors and operators in that basis, but now we have a set of rules to define the application of the operator to a state vector, i.e. the matrix multiplication:

$$\mathbf{M}\,|A\rangle = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \times \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = |B\rangle$$

Eigenvalues and eigenvectors

When we consider a linear operator, we can search for eigenvalues and eigenvectors (if they exist). Eigenvectors are vectors that don't change their direction when multiplied by the operator; their magnitude is scaled by a constant factor called the eigenvalue. Formally:

$$\mathbf{M}\,|\lambda\rangle = \lambda\,|\lambda\rangle$$

where $|\lambda\rangle$ is the eigenvector and λ the eigenvalue.

---

[8] The reason why we need this kind of operator will be clear in 1.3.2.

Considering the transformation between ket $|A\rangle$ and $|B\rangle$: $\mathbf{M}|A\rangle = |B\rangle$, taking into account the dual space of bras and searching for a machine that transforms the bra $\langle A|$ into $\langle B|$, we cannot simply use the matrix having as elements the complex conjugate of $\mathbf{M}$; the correct operator is the *Hermitian conjugate* of $\mathbf{M}$, which is the transpose of the matrix having as elements the complex conjugates of $\mathbf{M}$. We denote the Hermitian conjugate with the dagger †:

$$\mathbf{M}^\dagger = [\mathbf{M}^*]^T = [\mathbf{M}^T]^*.$$

We can now write:

$$\mathbf{M}|A\rangle = |B\rangle \Rightarrow \langle A|\mathbf{M}^\dagger = \langle B|.$$

An operator that is equal to its Hermitian conjugate is called a *Hermitian operator*. Formally, $\mathbf{M}$ is Hermitian if and only if

$$\mathbf{M} = \mathbf{M}^\dagger.$$

Hermitian operators have some important properties:

- all eigenvalues are real;
- eigenvectors form a *complete set*: all vectors obtained with the application of the operator can be expressed as a linear combination of eigenvectors;
- if λ_1 and λ_2 are different eigenvalues, the associated eigenvectors are orthogonal;
- if two eigenvalues are equal (*degeneracy*), it is always possible to find two associated eigenvectors that are orthogonal.

Fundamental theorem

The last three properties can be summed up in the following way:

Theorem 1. *The eigenvectors of a Hermitian operator form an orthonormal basis.*

1.3.2 Principles of quantum mechanics

Let's introduce the first four principles of quantum mechanics, the ones about observables[9].

Principles 1. *Observables in quantum mechanics are described by linear operators* **L**.

L must also be a Hermitian operator: we can consider this proposition an axiom itself or deduce it from the other principles.

Principles 2. *The results of a measurement can only be the eigenvalues associated with the observable operator.*

Calling λ_i a generic eigenvalue and $|\lambda_i\rangle$ the associated eigenvector, if the system is in the *eigenstate* $|\lambda_i\rangle$, the measurement always returns λ_i. Since all λ_i must be physical quantities they must be real, a peculiar property of Hermitian operators.

---

[9] The fifth, and last one, concerns the temporal evolution. It will be discussed later on (1.4).

Principles 3. *Unambiguously distinguishable states are represented by orthogonal vectors.*

Distinguishable states can be separated without ambiguity by a measurement. For example, if we want to distinguish between $|u\rangle$ and $|d\rangle$, we measure σ_z: *up* and *down* are distinct. We cannot, instead, say if a certain system is in state *up* or *right*, because even if the system is in the state $|u\rangle$ we can still measure σ_x and find (with 50% chance) that the system is in state $|r\rangle$.

Overlap

The inner product is a measure of how much two states are indistinguishable; for that reason it is also called overlap. Two states are physically distinct if the overlap is zero.

$$\langle u | d \rangle = 0$$
$$\langle u | r \rangle \neq 0$$

Principles 4. *If the system is in state $|A\rangle$ and we measure the observable* **L**, *the probability of obtaining λ_i is:*

$$P(\lambda_i) = \langle A | \lambda_i \rangle \langle \lambda_i | A \rangle .$$

where λ_i is a generic eigenvalue of **L** and $\langle \lambda_i |$, $|\lambda_i\rangle$ are the bra and ket associated with that eigenvalue (eigenvector of λ_i).

1.3.3 Spin Operator

The principles tell us what properties a machine must have to represent an observable. Let's construct the spin operator σ.

Until now, we have measured spins with the apparatus $\mathcal{A}$, orienting $\mathcal{A}$ along the component of our interest. σ is a mathematical tool that allows us to make predictions about the result of a measurement with $\mathcal{A}$ (fourth principle); as we can rotate $\mathcal{A}$, we must also rotate σ (mathematically). For this spatial property, σ is called a *3-vector operator*.

OPERATOR σ_z: Let's start with the simplest operator[10]. The second principle says that all eigenvectors of σ_z are $|u\rangle$ and $|d\rangle$, with associated eigenvalues $+1$ and -1. We can write this assertion as equations:

$$\sigma_z |u\rangle = |u\rangle$$
$$\sigma_z |d\rangle = -|d\rangle .$$

In matrix form:

$$\begin{pmatrix} (\sigma_z)_{11} & (\sigma_z)_{12} \\ (\sigma_z)_{21} & (\sigma_z)_{22} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$\begin{pmatrix} (\sigma_z)_{11} & (\sigma_z)_{12} \\ (\sigma_z)_{21} & (\sigma_z)_{22} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

The solution of this system is[11]:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

---

[10] This is because we have chosen $\mathscr{B} = \{ |u\rangle , |d\rangle \}$ as the basis.

[11] It is easy to verify that this operator is also linear.

OPERATOR σ_x: With the same reasoning, we can construct the operator along the x axis. We have already deduced the representations of *right* and *left* in equations 1.6 and 1.7 on page 10. The equations that allow us to construct σ_x are:

$$\begin{pmatrix} (\sigma_x)_{11} & (\sigma_x)_{12} \\ (\sigma_x)_{21} & (\sigma_x)_{22} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\begin{pmatrix} (\sigma_x)_{11} & (\sigma_x)_{12} \\ (\sigma_x)_{21} & (\sigma_x)_{22} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} = - \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} .$$

The solution of this system is:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} .$$

OPERATOR σ_y: The last direction is along the y axis. Considering the expressions for *in* and *out* given in equations 1.8 and 1.9 on page 10, and following the second principle, we can write:

$$\sigma_y |i\rangle = |i\rangle$$
$$\sigma_y |o\rangle = - |o\rangle .$$

We can rewrite this in matrix form, and the solution we would obtain is:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} .$$

Pauli matrices

We have obtained a matrix representation of the three spin operators σ_z, σ_x, and σ_y:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} . \tag{1.10}$$

These famous and important matrices are named after their inventor, Wolfgang Ernst Pauli.

1.3.4 Theory and experiments

Thanks to the operators σ_z, σ_x, and σ_y, if we know the state vector, we can statistically predict the result of a measurement of the spin along one of the three coordinate axes. What can we say about a measurement taken by orienting the apparatus $\mathcal{A}$ along a generic direction?

Considering $\mathcal{A}$ oriented along the unit vector $\hat{n}$, if σ behaves as a 3-vector, in order to obtain σ_n we only need the inner product:

$$\sigma_n = \vec{\sigma} \cdot \hat{n}$$

Expanding the components:

$$\sigma_n = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z .$$

If we choose the basis $\mathscr{B} = \{|u\rangle, |d\rangle\}$, we can use the Pauli matrices to express in matrix form the expression for σ_n:

$$\sigma_n = n_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + n_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + n_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}.$$

Given a direction (expressed by the unit vector $\hat{n}$), we can construct the matrix we have now made explicit, and then, after finding eigenvalues and eigenvectors, we can know all possible results of a measurement and obtain the probability associated with each result. For example, considering a direction in the x–z plane, the operator σ_n would be:

$$\sigma_n = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}$$

where θ is the angle between $\hat{n}$ and z. For this matrix, the eigenvalues and eigenvectors are:

$$\lambda_1 = 1 \qquad |\lambda_1\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$$

and

$$\lambda_2 = -1 \qquad |\lambda_2\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}.$$

It should be pointed out that the theory is in agreement with experimental results[12]. Eigenvalues are $+1$ and -1, exactly the only results that the apparatus $\mathcal{A}$ can retrieve. The probability of obtaining a certain result can be evaluated as:

$$P(+1) = |\langle u|\lambda_1\rangle|^2 = \cos^2\frac{\theta}{2}$$
$$P(-1) = |\langle u|\lambda_2\rangle|^2 = \sin^2\frac{\theta}{2}$$

Expectation value

Lastly, let's calculate the average value for the measurement σ_n. From the first experiment we have seen in 1.1.1, we already know that the result of repeated measurements with $\mathcal{A}$ is $\cos\theta$. Let's verify if our model is coherent with the world.

Expected values are obtained as:

$$\langle L\rangle = \sum_i \lambda_i P(\lambda_i)$$

Specifically:

$$\langle\sigma_n\rangle = (+1)\cos^2\frac{\theta}{2} + (-1)\sin^2\frac{\theta}{2} = \cos\theta.$$

This is in complete agreement with the experimental results.

Before going on, we present, without proof, a useful theorem about expectation values:

Theorem 2. *To know the expectation value of an observable, we can simply place the operator associated with the observable between the bra and ket of the state vector:*

$$\langle\mathbf{L}\rangle = \langle A|\mathbf{L}|A\rangle \tag{1.11}$$

where $\mathbf{L}$ is an observable, $|A\rangle$ is a state vector, and $\langle A|$ is the corresponding bra.

---

[12] If not, we must abandon this model and build another one.

1.3.5 Operator and Measure

Operators allow us to know the probability of measuring a certain spin given the direction of the measurement and the state vector. This probability is expressed by the state vector that we obtain when we apply the operator σ to the initial state.

It is important not to confuse the measurement act with the application of a machine that represents the observables. The spin state after the measurement is not the same as the one we obtain after the application of the operator. The operator is only an abstract mathematical construct that allows us to make statistical predictions about results, but doesn't have physical implications.

Let's consider an example to clarify the previous assertion. Having a spin prepared in the *up* state, its state vector is $|u\rangle = \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$. If we apply the operator σ_z, we would obtain again $\left(\begin{smallmatrix}1\\0\end{smallmatrix}\right)$, and if we measure the spin with $\mathcal{A}$ oriented along z, it will always display $+1$, and we conclude that the state after the measurement is $|u\rangle$.

Consider now a spin prepared *right*, i.e. $|r\rangle = 1/\sqrt{2}\,|u\rangle + 1/\sqrt{2}\,|d\rangle$. Applying again the operator σ_z, the new state vector is $1/\sqrt{2}\,|u\rangle - 1/\sqrt{2}\,|d\rangle$. This vector tells us the probability of measuring $\sigma_z = +1$ (50%), but it is not the spin state after the measurement. Using the apparatus $\mathcal{A}$, we could measure:

- $+1$: the final state will be *up*;
- -1: the final state will be *down*.

No matter the result of the measurement, the final state will be different from the one we obtained by applying the operator.

1.4 TEMPORAL EVOLUTION

Let's explore the laws that describe the temporal evolution of a quantum system. In particular, we will see how the state vector can evolve over time.

1.4.1 Unitarity

In classical mechanics we are used to having a motion law that links different states of our system deterministically; this means being able to know precisely the following state given the previous one. A good law, however, doesn't allow us only to know the future, but also the past states that brought the system to the current state[13].

Reversibility

In other words, we want physical transformations to be reversible. This requirement is so important that we call this property the *minus first law*, because it underlies everything else. If we think about the system states as nodes in an oriented graph, reversibility imposes that each node has exactly one input edge and one output edge. This fundamental law is also true in quantum mechanics and is called *unitarity*[14], and it assures us that no information is lost. The unitarity law can be expressed as:

---

[13] For example, if we observe a ball in free fall touching the floor with a certain speed and at a certain time, we can know exactly when and from what height the ball started its fall.

Axiom 3. *If two identical isolated systems are in different states, they stay in different states, and they were in different states in the past.*

1.4.2 Time-Development Operator

Considering a system in the state $|\Psi(t)\rangle$, where the t indicates that the state vector evolves over time, quantum motion equations allow us to obtain the state at time t given the initial state:

$$|\Psi(t)\rangle = \mathbf{U}(t)\,|\Psi(0)\rangle\,. \tag{1.12}$$

Determinism

Thanks to the operator $\mathbf{U}(t)$ we can know exactly the state vector $|\Psi(t)\rangle$ at time t, given $|\Psi(0)\rangle$. This assertion can be rephrased as:

Axiom 4. *The temporal evolution of the state vector is deterministic.*

Quantum mechanics is still non-deterministic, because knowing the state vector doesn't mean knowing the result of a measurement.

In order for $\mathbf{U}(t)$ to behave as we want, it has to:

- be a linear operator;
- respect reversibility.

The second constraint allows us to define the mathematical properties of $\mathbf{U}(t)$. Considering two initially different states $|\Psi(0)\rangle$ and $|\Phi(0)\rangle$, since there exists an experiment capable of certainly distinguishing the states, $|\Psi(0)\rangle$ and $|\Phi(0)\rangle$ must be orthogonal:

$$\langle \Psi(0)\,|\,\Phi(0)\rangle = 0.$$

Conservation of Distinctions

The minus first law assures that during the entire temporal evolution of the two systems, the state vectors $|\Psi(t)\rangle$ and $|\Phi(t)\rangle$ will continue to be distinguishable (orthogonal):

$$\langle \Psi(t)\,|\,\Phi(t)\rangle = 0 \qquad \forall t \geqslant 0.$$

If we rewrite this equation using formula 1.12, we obtain:

$$\langle \Psi(0)|\,\mathbf{U}^{\dagger}(t)\mathbf{U}(t)\,|\Phi(0)\rangle = 0.$$

From this we can see that $\mathbf{U}^{\dagger}(t)\mathbf{U}(t)$ must behave as the identity operator, that is:

$$\mathbf{U}^{\dagger}(t)\mathbf{U}(t) = \mathbf{I}. \tag{1.13}$$

An operator that behaves as $\mathbf{U}$ is *unitary*.

Principles 5. *The temporal evolution of state vectors is unitary.*

From the unitarity of $\mathbf{U}$ descends the *conservation of overlaps*: the overlap between two states (their inner product), subjected to the same temporal-development operator, is preserved over time.

---

[14] We will see in the next paragraph the reason for this name

1.4.3 The Hamiltonian

Often, in classical physics, a motion law is the result of a differential equation where we have exchanged a finite time interval with an infinite number of infinitesimal intervals.

Continuity

In quantum mechanics we can follow the same path and consider time intervals ϵ close to zero. In this scenario, after an ϵ amount of time, the state vector will change slightly and "smoothly", and the operator $\mathbf{U}(\epsilon)$ will be very similar to the identity. We can rewrite $\mathbf{U}(\epsilon)$ in order to highlight the difference with the identity $\mathbf{I}$ as:

$$\mathbf{U}(\epsilon) = \mathbf{I} - i\epsilon\mathbf{H}. \tag{1.14}$$

For now, i is a mere scale factor that later will help us recognize in $\mathbf{H}$ the quantum version of the classical Hamiltonian.

We can now express the infinitesimal evolution of a quantum system by combining equations 1.12 and 1.14:

$$|\Psi(\epsilon)\rangle = |\Psi(0)\rangle - i\epsilon\mathbf{H}\,|\Psi(0)\rangle\,.$$

Bringing to the left the time interval:

$$\frac{|\Psi(\epsilon)\rangle - |\Psi(0)\rangle}{\epsilon} = -i\mathbf{H}\,|\Psi(0)\rangle\,.$$

Now considering the limit for $\epsilon \to 0$, we can see in the left member the time derivative of the state vector:

$$\frac{\partial\,|\Psi(t)\rangle}{\partial t} = -i\mathbf{H}\,|\Psi(0)\rangle\,.$$

Before using $\mathbf{H}$ as the quantum Hamiltonian, we have to verify the dimensional correctness. As in classical mechanics, the Hamiltonian is the mathematical construct that represents the energy. In our formula, however, ignoring the state vector, we have the inverse of time on the left and the energy on the right. To resolve this problem, let's introduce an important physical constant: the reduced Planck constant, $\hbar$.

The equation becomes:

Time-dependent Schrödinger equation

$$\hbar\frac{\partial\,|\Psi\rangle}{\partial t} = -i\mathbf{H}\,|\Psi\rangle \qquad \text{or} \qquad \frac{\partial\,|\Psi\rangle}{\partial t} = \frac{-i\mathbf{H}\,|\Psi\rangle}{\hbar}. \tag{1.15}$$

The constant $\hbar$ has units of ${}^{\mathrm{kg}\cdot\mathrm{m}^2}/_{\mathrm{s}}$ and resolves the incompatibility between the two members. This equation is fundamental and is called the *generalized Schrödinger equation*, or time-dependent Schrödinger equation. If we know the Hamiltonian of an undisturbed system, we can know the evolution of the state vector.

If $\mathbf{H}$ represents the energy of the system, we should be able to measure it, so $\mathbf{H}$ has to be an observable. If $\mathbf{H}$ is an observable, it must be a Hermitian operator; let's verify it. Starting from 1.13 and substituting $\mathbf{U}$ with 1.14, we obtain:

$$(\mathbf{I} + i\epsilon\mathbf{H}^\dagger)(\mathbf{I} - i\epsilon\mathbf{H}) = \mathbf{I}.$$

Expanding to first order in ϵ, we find:

$$\mathbf{H}^\dagger - \mathbf{H} = 0 \Rightarrow \mathbf{H}^\dagger = \mathbf{H}.$$

We have concluded that $\mathbf{H}$ is an Hermitian operator that represents an observable: the energy of the system. Eigenvalues of $\mathbf{H}$ are the results of all possible direct measurements of the energy of the system.

Quantum Hamiltonian

1.4.4 Commutators

In a system that evolves with time, we expect that the expectation values for a certain observable $\mathbf{L}$ will also change. Thanks to equation 1.11 on page 15, we can write explicitly the time dependence of expectation values:

$$\langle \mathbf{L} \rangle = \langle \Psi(t) | \mathbf{L} | \Psi(t) \rangle .$$

The time derivative[15] is:

$$\frac{d}{dt} \langle \Psi(t) | \mathbf{L} | \Psi(t) \rangle = \left\langle \dot{\Psi}(t) \middle| \mathbf{L} \middle| \Psi(t) \right\rangle + \left\langle \Psi(t) \middle| \mathbf{L} \middle| \dot{\Psi}(t) \right\rangle .$$

Substituting bra and ket with the time-dependent Schrödinger equation 1.15 (namely $\left|\dot{\Psi}(t)\right\rangle = \frac{-i}{\hbar} \mathbf{H} \left|\Psi(t)\right\rangle$), we obtain:

$$\frac{d}{dt} \langle \Psi(t) | \mathbf{L} | \Psi(t) \rangle = \frac{i}{\hbar} \langle \Psi(t) | \mathbf{HL} | \Psi(t) \rangle - \frac{i}{\hbar} \langle \Psi(t) | \mathbf{LH} | \Psi(t) \rangle .$$

That can be rewritten as:

$$\frac{d}{dt} \langle \Psi(t) | \mathbf{L} | \Psi(t) \rangle = \frac{i}{\hbar} \langle \Psi(t) | [\mathbf{H}, \mathbf{L}] | \Psi(t) \rangle .$$

The quantity $\mathbf{HL} - \mathbf{LH}$ is called the *commutator*, and since, in general, the product between operators (matrices) is not commutative, the commutator is not zero (when it is zero, we say that $\mathbf{H}$ and $\mathbf{L}$ commute). Commutators are important in physic, and the commutator between two operators, in this case $\mathbf{H}$ and $\mathbf{L}$, is denoted by:

$$\mathbf{HL} - \mathbf{LH} = [\mathbf{H}, \mathbf{L}].$$

With the commutator we can express concisely the derivative of the expectation value for the observable $\mathbf{L}$:

$$\frac{d}{dt} \langle \mathbf{L} \rangle = \frac{i}{\hbar} \langle [\mathbf{H}, \mathbf{L}] \rangle \tag{1.16}$$

or equivalently:

$$\frac{d}{dt} \langle \mathbf{L} \rangle = -\frac{i}{\hbar} \langle [\mathbf{L}, \mathbf{H}] \rangle . \tag{1.17}$$

This equation links variations of the expectation values of an observable ($\mathbf{L}$) to the expectation values of another physical observable ($-\frac{i}{\hbar}[\mathbf{L}, \mathbf{H}]$)[16].

---

[15] Derivative of a product: $\mathbf{L}$ doesn't depend on time and the dot denotes the time derivative (Newton notation).

[16] It is possible to demonstrate that if $\mathbf{L}$ and $\mathbf{H}$ are Hermitian, then $[\mathbf{L}, \mathbf{H}]$ is also Hermitian.

1.4.5 Conservation of Energy

In quantum mechanics, when we say that a quantity is conserved, we mean that the expectation value of that quantity doesn't change. If we look at equation 1.17, the condition for the expectation value not to change is that the commutator between this quantity and the Hamiltonian is zero. It is possible to demonstrate that:

Theorem 3. *Having an observable* $\mathbf{Q}$*, if* $[\mathbf{Q}, \mathbf{H}] = 0$*, then every power satisfies* $[\mathbf{Q}^n, \mathbf{H}] = 0$*. This means that the expectation value* $\langle Q \rangle$ *is conserved, and any power of the expectation value* $\langle Q^n \rangle$ *does not change with time.*

The most obvious quantity that is conserved is the Hamiltonian **H** and, since every operator commutes with itself, we always have:

$$[\mathbf{H}, \mathbf{H}] = 0.$$

We can conclude that, under very general conditions, energy is conserved in quantum mechanics.

1.5 CONCLUSIONS

We conclude this chapter with a recap of what we have discovered in these pages, trying to put everything together to answer the question that opened this chapter: what are the physical limits of quantum computing, and why must our algorithms be reversible?

We started the chapter with an experiment that shows that quantum mechanics is not deterministic. We can, however, make some predictions if we consider the expectation value of a measurement instead of a single result.

We have built state vectors and understood their mathematical meaning, focusing on the fact that knowing the state vector doesn't allow us to know the result of a measurement. We have defined the inner product between state vectors, observed that it is a measure of the overlap between states, and concluded that two distinguishable states must be orthogonal.

We have linked a state vector to the result of a measurement –to be precise, to the average of the results of multiple measurements– with machines, Hermitian operators that represent observables. We have built the spin operator and used it to predict the result of a simple experiment, showing how the theory we have built so far is in accordance with experimental results.

Our introduction continues with the analysis of the temporal evolution of a quantum system. We have described the evolution of a state vector with an unitary operator; the application of this operator to a state vector produces the new state in which the system will be. We understood that the temporal evolution of the state vector is deterministic and that indeterminacy is caused only by the act of measuring.

Considering infinitesimal time intervals, we have deduced the time-dependent Schrödinger equation and, thanks to this equation, we have shown how to describe the temporal evolution of expectation values for a certain observable. During this analysis, we also introduced the Hamiltonian of the system, a Hermitian operator that describes the energy of the system.

The discussion ends with a comforting result: as in classical physics, the energy of a closed system is conserved. We have obtained this result by presenting the commutator and linking the temporal evolution of an observable with the commutator between the observable and the Hamiltonian (energy) of the system. The commutator of the Hamiltonian with itself is trivially zero, so the expectation value for the energy doesn't change.

All the information that we have learned allows us to understand the constraint of writing only reversible algorithms for quantum-gate-based quantum computers. Quantum gates operate on qubits through physical transformations[17]. These transformations, like all transformations in quantum mechanics, are described by unitary operators that are intrinsically reversible. This means that all quantum gates are reversible.

In other words, we can build only quantum gates that, having as input different (distinguishable) states, return orthogonal states; also, due to the conservation of overlaps, the inner product between input states is conserved during the quantum gate transformation.

Reversibility doesn't mean that we can go forward and backward in time as we please, but that all quantum gates express injective functions: if we know the output, we can know the input, or in more physical terms, if we know the final state of qubits[18] and the transformations applied to this system (i.e., those implemented by the quantum gates), we can determine the initial state.

Since every quantum algorithm has to be implemented as a path through quantum gates, and every quantum gate is reversible, the algorithms as a whole must also be reversible.

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[17] How depend strongly on the particular physical implementation.

[18] This is a complex system (composed of more than one qubit); to fully understand these systems, we should take into account entanglement. Since our discussion is already quite long, and the temporal evolution of an entangled system is still unitary (reversible), we exclude entanglement from our introduction.

2

QUANTUM GATE

3 QUANTUM ANNEALING

4 ONTOLOGY

In this chapter we explain what kind of knowledge base (KB) an ontology is, how to build an ontology, and why this knowledge representation is important. To clarify and demonstrate why ontologies are useful, we present an example of an important ontology, briefly discussing its utility.

The rest of the chapter is about reasoning on ontologies; we discuss the semantics of the formal language used to represent knowledge, what we mean when saying interpretation of a KB, and the complexity of finding an interpretation.

4.1 KNOWLEDGE BASE

In the field of information technologies, an ontology is a structured representation of knowledge about a certain domain of interest; however, the study of knowledge began much before informatics. To better understand what an ontology is, let's start with the philosophical definition and then point out the differences between this vision and the IT one.

4.1.1 Ontology in philosophy

Ontology was born as a branch of philosophy. In this context it is the science of what is, of the kinds and structures of objects, properties, events, processes, and relations in every area of reality[1].

The goal of an ontology is to give a definitive and exhaustive classification of entities in all spheres of being. With the term "definitive" we mean that an ontology should answer questions such as: "What classes of entities are needed for a complete description and explanation of all the goings-on in the universe?" With the term "exhaustive", instead, we mean that all types of entities and relations between these entities are included in our ontology[1].

4.1.2 Ontology in computer science

Thanks to the advent of the internet and the development of bigger and bigger software used by bigger and bigger groups of users, what we might call the Tower of Babel problem emerged. Each research group develops its KB with terms and concepts shared and accepted only inside the group. For example, different databases may use identical labels but with different meanings, and the same meaning may be expressed with different names[1].

To address the incompatibility problem between software, databases, and research groups, ontologies have become an important research topic in computer science where the goal is to define standards for data exchange, information integration, and interoperability[2].

In this field the term ontology gains a new meaning:

Definition 1. *Ontologies represent a formal and explicit specification of a shared conceptualization[3].*

In this definition the keywords are:

- CONCEPTUALIZATION an ontology creates an abstract model identifying and defining only the relevant concepts;
- EXPLICIT the types of concepts and constraints on their use are explicitly defined;
- FORMAL an ontology should be machine-readable;
- SHARED the knowledge represented by the ontology has to be accepted by a group of people, ideally by everyone.

When we use an ontology to represent knowledge we are describing a graph where entities are bound together through relationships, and classified according to a formal description of the world[4]. Knowledge bases expressed with this formalism are divided into two components[5]:

- T-BOX stores a set of universally quantified assertions (inclusion assertions) stating general properties of concepts and roles;
- A-BOX contains assertions on individual objects (instance assertions).

We can see some similarities between an ontology and a database: the T-Box can be seen as the Entity-Relation schema and the A-Box as the set of all entries of the database. There is, however, a logical difference between the world represented by an ontology and the world represented by a database.

Databases make the *closed world assumption*: everything that is not present in the database is automatically false; for example, if a person does not appear in a bank registry it means that that person is not a client of the bank.

Ontologies, on the other hand, make the *open world assumption*[6], which means, for example, that we can assert that a certain person is a parent even if we have not specified any son or daughter.

4.1.3 OWL Language

OWL 2 Web Ontology Language is an ontology language for the Semantic Web with a formally defined meaning[7]. Thanks to OWL we can model classes and relations between classes (T-Box) and individuals with their specific properties and relations between individuals (A-Box). The T-Box is the conceptualization of the world, while the A-Box is a certain instance of the world we have modelled in the T-Box.

OWL is a declarative language and defines the state of the world in a logical way. In particular, we are interested in OWL DL where the meaning of ontologies expressed with this language is assigned in a Description Logic style. OWL DL is, therefore, decidable and an appropriate tool (so-called reasoner) can then be used to infer further information about that state of the world[7].

OWL per se doesn't specify any syntax, it states only what can or cannot be expressed in an ontology. The World Wide Web Consortium (W3C) standardizes various syntaxes, some inspired by functional languages, others more suitable for storing on web pages. The only syntax that must be implemented by all tools to be compliant with the OWL standard is the RDF/XML syntax[7] (examples of this syntax are provided in 4.2.1).

4.1.4 Importance of ontologies

Ontologies are important in various fields, from interoperability to machine learning.

In the Semantic Web context, ontologies are a main vehicle for data integration, sharing, and discovery[8]. Different research groups can use the same ontology to share a unified vocabulary that helps build common knowledge and helps to better integrate the results obtained by each group.

In a more commercial scenario, an ontology can be used as a translation layer between different databases or software that are built by different teams and use different vocabularies.

In the machine learning field an ontology could be used to support the sharing and reuse of formally represented knowledge among AI systems[3]. In the last years, we have become used to training AI agents on unstructured data, but formal knowledge can help to fine-tune these models or to check their answers.

4.2 EXAMPLE ONTOLOGIES

To help understanding the structure of ontologies and to show a practical example of ontology, we present two ontologies: a simple ontology about family relationships and DOLCE, a foundational ontology.

4.2.1 Simple ontology

This simple ontology about parental relationships shows the basic structure of an ontology, helping to understand the graph structure of these KBs and the relations between the T-Box and A-Box.

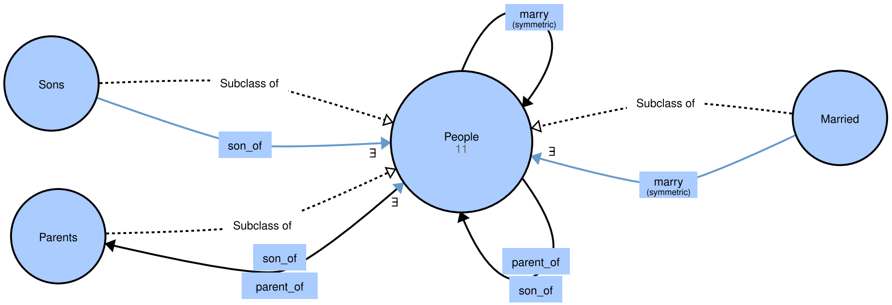


Figure 4.1: Graph for T-Box

In figure 4.1, we can see the T-Box of the ontology: this structure specifies what our domain of interest is, and what entities could possibly populate our world. This ontology is about people, so the main class/concept is `People`: this class has several subclasses that represent parents, children, and married people. We can assert that a person belongs to the married class without specifying the partner (open world assumption) but we can also infer that a person belongs to the parents class because we have created a relationship of type `parent_of` between that person and another person.

OWL allows us to express rules to infer when a member of a class belongs also to another class. The following code shows (in the RDF/XML syntax) the definition of the class `Parent`[1]:

```
1 <owl:Class rdf:about="http://people#Parent">
2   <owl:equivalentClass>
3     <owl:Restriction>
4       <owl:onProperty rdf:resource="http://people#parent_of"/>
5       <owl:someValuesFrom rdf:resource="http://people#Person"/>
6     </owl:Restriction>
7   </owl:equivalentClass>
8   <rdfs:subClassOf rdf:resource="http://people#Person"/>
9 </owl:Class>
```

Listing 1: Definition of parents

At line 8 we can see that `Parent` is a subclass of `People`, and at lines 4 and 5 it is specified that a parent is a person that is `parent_of` another person.

From figure 4.1 we can also see some properties of the relations:

- relation `marry` is symmetric;
- relation `parent_of` is the inverse of `son_of`;
- we can specify a domain and a range for relations.

OWL gives us constructs for all of these specifications (and other more complex ones).

Now we can populate the ontology by adding individuals and relations between individuals. For this small example we take inspiration from the Simpson family, and in the family tree on the right we can see the small portion of the family represented. To show what we mean by open world assumption we have asserted that Jackie is a married person even if in our representation there is no husband.

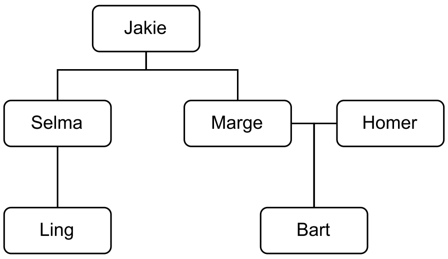


Figure 4.2: Simpson family tree

Our ontology covers a small domain, the types of entities that populate our model are very limited; the next example shows the commitment of engineering an ontology to represent virtually anything in the universe.

---

[1] The complete code of the ontology can be seen at `url`.

4.2.2 DOLCE ontology

DOLCE (Descriptive Ontology for Linguistic and Cognitive Engineering) is a top-level (foundational) ontology[9]; this means that this ontology describes fundamental aspects of reality and should be used as a base for constructing an ontology about a particular domain of interest. For this reason DOLCE defines only the T-Box; the user will then expand the T-Box with specific classes and relations of interest, and lastly will populate the A-Box.

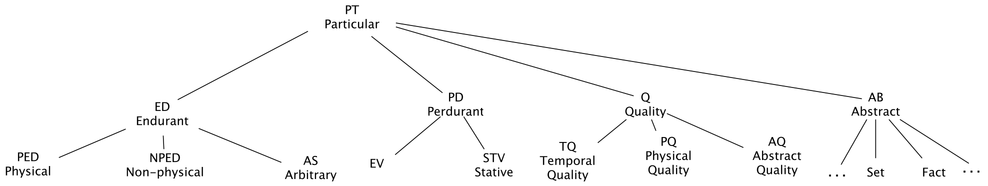


Figure 4.3: First layer of DOLCE taxonomy

STRUCTURE OF DOLCE: in DOLCE we can model the modification of objects during time; for this reason DOLCE distinguishes between endurants and perdurants. Endurants may acquire and lose properties and parts through time, perdurants are fixed in time[9]. With a simplification we can see endurants as the physical entities that are modified by the passing of time (like objects, animals, and people) and perdurants as events that, once they have passed, cannot be changed anymore (like a tennis match or a conference).

The relation connecting endurants and perdurants is called participation. A physical entity can be in time by participating in a perdurant, and perdurants happen in time by having endurants as participants[9].

Another important aspect of DOLCE is the way we attribute a property to an entity; this is done by using qualities, which are what can be perceived and measured. To do so we can assert that a certain entity has a specific quality and then, when it is possible, quantify that quality.

IMPORTANCE OF DOLCE: foundational ontologies can be useful in several fields, from conceptual modeling to natural language processing. DOLCE, today, is used in a variety of domains where it provides the general categories and relations needed to give a coherent view of reality[9].

4.3 RERASONING ON ONTOLOGY

In 4.1.3 we have introduced the standard language to encode an ontology; in order to infer new information, starting from the one we already have, we need to better specify the semantics of OWL DL.

4.3.1 $\mathcal{SROIQ}$ DL

The semantics of OWL DL extends the semantics of the description logic (DL) $\mathcal{SROIQ}$ to provide support for datatypes and punning[10]. For constructs available both in OWL DL and in $\mathcal{SROIQ}$ the semantics correspond exactly.

Description logics allow the modeling of the domain of interest with three kinds of entity: concepts, roles, and individual names. These entities correspond to unary predicates, binary predicates, and constants in first-order logic[6]. From the point of view of ontology and OWL, concepts are classes, roles are relationships, and individual names are the individuals that can belong to one or more classes.

$\mathcal{SROIQ}$ is one of the most expressive description logics where we have constructors for:

- transitive roles: $\mathcal{S}$
- role inclusions, local reflexivity, universal role, symmetry, asymmetry, role disjointness, reflexivity, and irreflexivity: $\mathcal{R}$;
- nominals: $\mathcal{O}$;
- inverse roles: $\mathcal{I}$;
- qualified number restrictions: $\mathcal{Q}$.

For example, we can construct the ontology shown in figures 4.1 and 4.2 with a set of assertions like:

`person(selma)` `married(jackie)` `parent_of(marge, bart)`

Each of these statements is called an axiom and the set of all axioms constitutes our KB.

4.3.2 Interpretation of a knowledge base

An interpretation I consists of a domain Δ^I and an interpretation function $\cdot^I$ that maps:

$$\text{concept } A \rightarrow A^I \subseteq \Delta^I$$
$$\text{role } R \rightarrow R^I \subseteq \Delta^I \times \Delta^I$$
$$\text{named individual } a \rightarrow a^I \in \Delta^I$$

In other words I assigns a fixed meaning to all entities in the KB[6]. By having a fixed meaning, we can say if an axiom α holds in I or not; in the first case we say that I satisfies α and we write $I \models \alpha$.

If all axioms in an ontology are satisfied by I we say that I is a *model* of the ontology. An ontology is consistent if it accepts at least one model.

A reasoner should at least be capable of saying if an ontology is consistent, but we are also interested in querying knowledge to retrieve new information.

QUERY INTERPRETATION: Considering a KB K, a query q consists of axiom templates where $\mathcal{SROIQ}$ axioms are composed of concept names, role names, and individual names, but also of concept variables, role variables, and individual variables. A solution for the query is an interpretation μ that allows us to rewrite all variables in q with names; we denote with $\mu(q)$ the result of the substitution.

The evaluation of q over K is a set of solutions μ with:[11]

$$\{\ \mu | K \cup \mu(q) \text{ is a } \mathcal{SROIQ} \text{ knowledge base and } K \models \mu(q)\}$$

In other words μ binds all free variables of q to names present in K[11].

A naive approach to find the solution to a query is to simply test for each possible solution mapping μ, if $K \models \mu(q)$; however, in the worst case, the number of mappings that have to be tested is exponential in the number of variables in the query[11].

4.3.3 Complexity of reasoning

Since presenting an actual algorithm for reasoning on ontologies is out of the scope of this work, we only give some hints about the reasons for the complexity and then present the theoretical results.

It is easy to convince oneself that the more axioms there are in an ontology, the fewer interpretations exist that satisfy all axioms. On the other hand, if an ontology has fewer models, the more axioms hold in all of them and the more logical consequences follow from the ontology.

We can rephrase these two statements by saying that the semantics of description logics are *monotonic*: the more knowledge we embed in an ontology, the more results it returns[6].

A more formal view is given in [12], where two *sources of complexity* are identified:

- OR-branching: the presence of disjunctive constructors;
- AND-branching: the presence of qualified existential and universal quantifiers.

The AND-branching is responsible for the exponential size of a single interpretation, and the OR-branching is responsible for the exponential number of different interpretations.

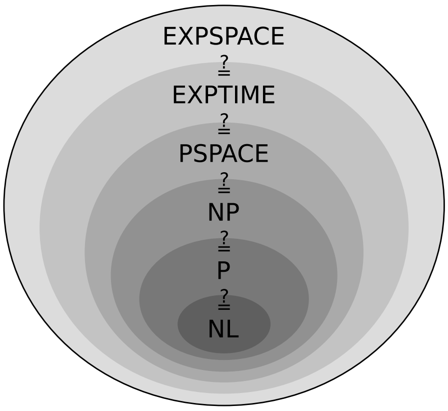


Figure 4.4: Complexity classes

To discuss the complexity of reasoning we take into account the description logic $\mathcal{ALC}$; this DL is a restriction of $\mathcal{SROIQ}$[6], so its complexity is a lower bound for $\mathcal{SROIQ}$. It is possible to prove the PSpace-hardness of satisfiability in $\mathcal{ALC}$[12], therefore also $\mathcal{SROIQ}$ DL is at least PSpace-hard.

This result shows that, unless PSpace = PTime, the exponential time complexity of any algorithm that makes inference on an ontology cannot be improved .

For those interested in some numerical examples to better understand what this class of complexity means in a real context, [13] presents the reasoner HermiT[2] and evaluates its performance on some real ontologies.

4.4 CONCLUSIONS

In this chapter we have explained what an ontology is and we have motivated the interest in this field. We have shown both theoretically and with examples what can be expressed in an ontology and what cannot. We have formally defined what the interpretation of a KB is and showed what a query and its results are.

Lastly, we have characterized the complexity of reasoning on ontologies. This complexity is what motivated us to search for other paradigms to infer new knowledge starting from an ontology. In the next chapters we will build the tools necessary to achieve this goal.

---

[2] `http://www.hermit-reasoner.com/`.

Part II

TOOLS

5 ENVIRONMENT SETUP

In this chapter we describe the environment, libraries and tools we use to execute our tests.

In the following sections we install the SDKs to develop and interact with quantum computers from IBM and D-Wave. We also present two other useful tools to easily write optimization problems.

5.1 PYTHON ENVIRONMENT

The language used to interface with quantum computers is usually Python. In this section we create a virtual environment in Python in order to communicate with the IBM quantum computer and the D-Wave quantum computer.

For our tests we manage Python environments with `conda`. Let's start by creating the virtual environment named `quantum` and activating it with:

```
conda create --name quantum python=3.12 pip
conda activate quantum
```

For our tests and to follow the various examples presented both by IBM and D-Wave, it is also useful to be able to run a Jupyter notebook. We can install Jupyter with:

```
pip install jupyter
```

5.2 IBM QISKIT

To program a gate-based architecture and to access IBM quantum computers we use the *Qiskit* software stack. The name Qiskit is a general term referring to a collection of softwares for executing programs on quantum computers.

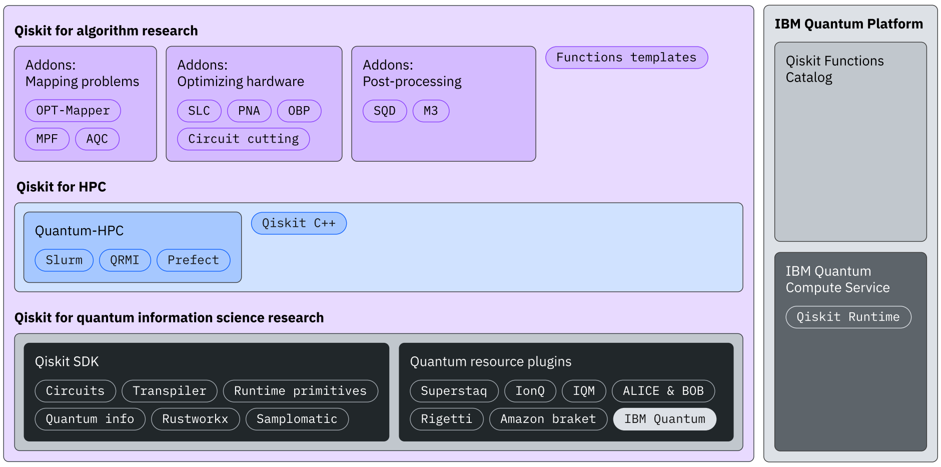

Qiskit for algorithm research
Addons: Mapping problems
OPT-Mapper
MPF
AQC
Addons: Optimizing hardware
SLC
PNA
OBP
Circuit cutting
Addons: Post-processing
SQD
M3
Functions templates
Qiskit for HPC
Quantum-HPC
Slurm
QRMI
Prefect
Qiskit C++
Qiskit for quantum information science research
Qiskit SDK
Circuits
Transpiler
Runtime primitives
Quantum info
Rustworkx
Samplomatic
Quantum resource plugins
Superstaq
IonQ
IQM
ALICE & BOB
Rigetti
Amazon braket
IBM Quantum
IBM Quantum Platform
Qiskit Functions Catalog
IBM Quantum Compute Service
Qiskit Runtime

Figure 5.1: Qiskit software stack

The core components are *Qiskit SDK* and *Qiskit Runtime*. The first one is completely open source and allows the developer to define his circuit; the second one is a cloud-based service for executing quantum computations on IBM quantum computers.

5.2.1 Hello World

Following the IBM documentation[1] we can install the SDK and the Runtime with:

```
1 pip install qiskit matplotlib qiskit[visualization]
2 pip install qiskit-ibm-runtime
3 pip install qiskit-aer
```

Line 3 installs Aer, which is a high-performance simulator for quantum circuits written in Qiskit. Aer includes realistic noise models, and we will use it later to test our circuit.

Sometimes the Qiskit stack suffers from incompatibilities between the various software components that compose the environment. At the moment of writing, the latest packages seem to work without any problem. For our tests we will use `qiskit: 2.2.3`, `qiskit-ibm-runtime: 0.43.1` and `qiskit-aer: 0.17.2`.

If the setup is successful we are now able to run a small test to build a Bell state (two entangled qubits). The following code assembles the gates, shows the final circuit and uses a sampler to simulate on the CPU the result of 1024 runs of the program.

```python
from qiskit import QuantumCircuit
from qiskit.primitives import StatevectorSampler

qc = QuantumCircuit(2)
qc.h(0)
qc.cx(0, 1)
qc.measure_all()

sampler = StatevectorSampler()
result = sampler.run([qc], shots=1024).result()
print(result[0].data.meas.get_counts())
qc.draw("mpl")
```

Listing 2: Building Bell state

5.2.2 Transpilation

Each Quantum Processing Unit (QPU) has a specific topology. We need to rewrite our quantum circuit in order to match the topology of the selected device on which we want to run our program. This phase of rewriting, followed by an optimization, is called transpilation.

---

[1] https://quantum.cloud.ibm.com/docs/en/guides/install-qiskit

Considering, for now, a fake hardware (so we do not need an API key) we can transpile the quantum circuit `qc`, from the code above, to match the topology of a specific QPU:

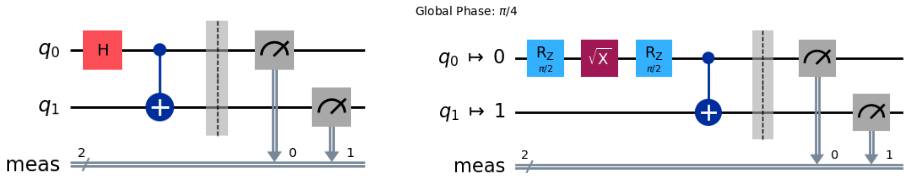
```python
from qiskit_ibm_runtime.fake_provider import FakeWashingtonV2
from qiskit.transpiler import generate_preset_pass_manager

backend = FakeWashingtonV2()
pass_manager = generate_preset_pass_manager(backend=backend)

transpiled = pass_manager.run(qc)
transpiled.draw("mpl")
```

Listing 3: Transpilation

The following picture shows (5.2a) the quantum circuit that builds a Bell state, and (5.2b) the transpiled version where the Hadamard gate is replaced to match the actual topology of the QPU.



(a) Original circuit **(b)** Transpiled circuit

Figure 5.2: Transpilation example

5.2.3 Execution

To test our transpiled circuit we use Aer, which allows us to simulate also the noise of real quantum hardware. We can execute our program with:

```python
from qiskit_aer.primitives import SamplerV2

sampler = SamplerV2.from_backend(backend)
job = sampler.run([transpiled], shots=1024)
result = job.result()
print(f"counts for Bell circuit : {result[0].data.meas.get_counts()}")
```

Listing 4: Simulated execution

If we look at the results of the execution we can observe that some answers present non-entangled qubits; this is caused by the (simulated) noise of the quantum device. A typical output of the execution could be:

```
> counts for Bell circuit : {'00': 504, '11': 503, '01': 10, '10': 7}
```

Where states `01` and `10` should not be present in an ideal execution with no errors.

5.2.4 A complete example on real hardware

5.3 D-WAVE OCEAN

To define an optimization problem that can be solved on a D-Wave quantum computer we use the Ocean software stack. Ocean also allows us to interact with D-Wave hardware, submit a problem, and simulate the execution on a classical CPU.

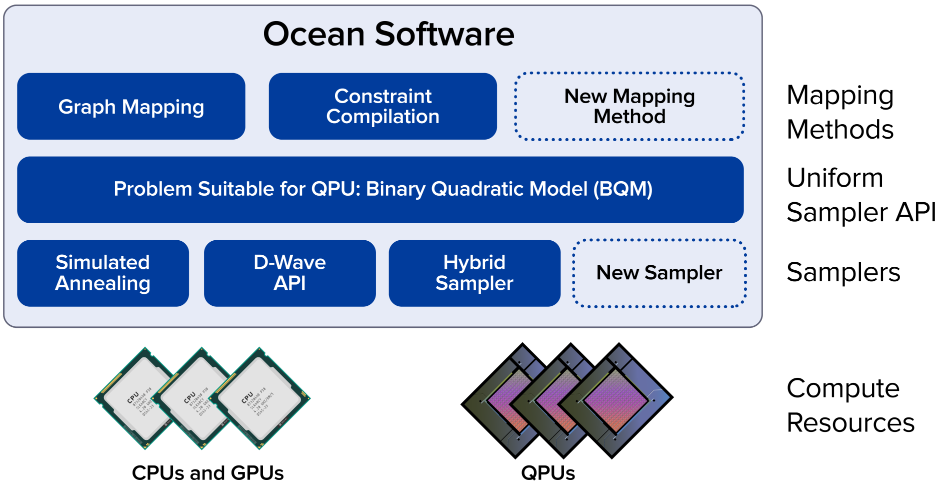

Ocean Software
Graph Mapping
Constraint Compilation
New Mapping Method
Mapping Methods
Problem Suitable for QPU: Binary Quadratic Model (BQM)
Uniform Sampler API
Simulated Annealing
D-Wave API
Hybrid Sampler
New Sampler
Samplers
CPUs and GPUs
QPUs
Compute Resources

Figure 5.3: Ocean software stack

All tools that implement the steps needed to solve your problem on a CPU, a D-Wave quantum computer, or a quantum-classical hybrid solver can be installed with:

```
pip install dwave-ocean-sdk
```

After the installation, running the command `dwave setup` will start an interactive prompt that guides us through a full setup. During the setup it is also possible to add an API token or connect to the D-Wave account to import a key directly to use the quantum hardware.

5.3.1 Hello World

To present a simple optimization program we consider the minimum vertex cover (MVC) problem. Given a graph $G = (V, E)$, the problem asks to find a subset $V' \subseteq V$ such that, for each edge $\{u, v\} \in E$, at least one of u or v belongs to V', and the number of nodes in V' ($|V'|$) is the lowest possible.

The reduction from MVC to an Ising formulation is well known. The cost function that we want to minimize can be expressed by:

$$\text{cost} = \sum_{i=1}^{|V|} v_i + 2 \cdot \sum_{\{i,j\} \in E} (1 - v_i - v_j + v_i v_j)$$

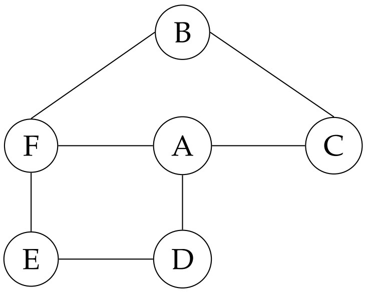
where $v_i \in \{-1, 1\}$ and $v_i = 1$ means that $v_i \in V'$, otherwise $v_i = -1$.

Like all problems in Ising form we can express the cost as a symmetric matrix, so our function becomes

$$\text{cost} = v^{\mathsf{T}} \times \mathbf{M} \times v$$

where v is the vector containing the binary variables v_i.

The figure shows an example graph (5.4a) and the corresponding matrix (5.4b) expressing the cost function.



(a) Original graph

$$\mathbf{M} = \begin{pmatrix} 1 & 0 & 2 & 2 & 0 & 2 \\ 0 & 1 & 2 & 0 & 0 & 2 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

(b) Corresponding matrix

Figure 5.4: Ising formulation

The following code presents a possible implementation of the Ising model described above. We have defined two dictionaries to store the matrix coefficients. The last line of code finds ten possible answers to the problem using the simulated annealing function implemented by D-Wave.

```python
from dwave.samplers import SimulatedAnnealingSampler
linear = {'A': 1, 'B': 1, 'C': 1, 'D': 1, 'E': 1, 'F': 1}
quadratic = {('B', 'C'): 2, ('B', 'F'): 2, ('C', 'A'): 2, ('D', 'A'): 2,
↪  ('E', 'D'): 2, ('E', 'F'): 2, ('F', 'A'): 2}
sampler = SimulatedAnnealingSampler()
result = sampler.sample_ising(linear, quadratic, num_reads=10)
```

Listing 5: Ising example

If we print the results with `print(result.aggregate())` we can observe something similar to this:

```
  A  B  C  D  E  F energy num_oc.
0 -1 -1 +1 +1 -1 +1  -14.0       6
1 +1 +1 -1 -1 +1 -1  -14.0       4
['SPIN', 2 rows, 10 samples, 6 variables]
```

The two different results represent the two correct answers to our particular instance of the MVC problem.

5.3.2 Example on real hardware

5.3.3 Minor embedding

5.4 PYQUBO AND QUBOVERT

In listing 5 we have manually built the matrix representing the function that we want to minimize. It can be useful to have some tools that allow us to work at a higher level, defining cost functions like **??** that we defined in the section about quantum annealing (**??**).

Considering again the MVC problem, the objective function tends to minimize the number of nodes in our subset, while the penalty increases the cost if we leave out some edges. This interpretation allows us to transform the Ising model into the more familiar —from the point of view of a computer scientist— QUBO model, where all variables $x_i \in \{0, 1\}$. Let's see how PyQUBO and qubovert help us in this task.

5.4.1 PyQUBO

Reading from the documentation on the PyQUBO site[2], PyQUBO allows us to create QUBOs or Ising models from flexible mathematical expressions easily. Some of the features of PyQUBO are:

- Python based (C++ backend);
- Fully integrated with Ocean SDK;
- Automatic validation of constraints;
- Placeholder for parameter tuning.

We can install PyQUBO with `pip install pyqubo` and rewrite our MVC problem by defining the Hamiltonian that we want to minimize.

```
from pyqubo import Binary, Placeholder, Constraint
from dwave.samplers import SimulatedAnnealingSampler

A, B, C, D, E, F  = Binary('A'), Binary('B'), Binary('C'), Binary('D'),
↪  Binary('E'), Binary('F')

H_objective = (A + B + C + D + E + F)
H_penalty = Constraint(((1 - A - C + A*C) +\
(1 - A - D + A*D) +\
(1 - A - F + A*F) +\
(1 - B - C + B*C) +\
(1 - B - F + B*F) +\
(1 - D - E + D*E) +\
(1 - E - F + E*F)) ,label='cnstr0')

L = Placeholder('L')
H = H_objective + L*H_penalty
H_internal = H.compile()
bqm = H_internal.to_bqm(feed_dict={'L': 2})

sampler = SimulatedAnnealingSampler()
result = sampler.sample(bqm, num_reads=10)
```

Listing 6: Rewriting MVC with pyQUBO

---

[2] https://pyqubo.readthedocs.io/en/latest/

Listing 6 presents a possible re-implementation of listing 5, where we also see how PyQUBO interfaces with the Ocean SDK (line 17), and how to create (lines 14–16) and instantiate (line 17) a parametric Hamiltonian.

5.4.2 qubovert

As written in the documentation[3], qubovert is the one-stop package for formulating, simulating, and solving problems in boolean and spin form. Using our nomenclature, boolean and spin form are respectively QUBO and Ising form.

Qubovert allows us to define various types of optimization problems that can be solved by brute force, with qubovert's simulated annealing, or with D-Wave's solver. Models defined in qubovert are:

- **QUBO:** Quadratic Unconstrained Boolean Optimization;
- **QUSO:** Quadratic Unconstrained Spin Optimization (Ising model);
- **PUBO:** Polynomial Unconstrained Boolean Optimization;
- **PUSO:** Polynomial Unconstrained Spin Optimization;
- **PCBO:** Polynomial Constrained Boolean Optimization;
- **PCSO:** Polynomial Constrained Spin Optimization.

In addition to generic models, qubovert has a library of famous NP-complete problems mapped to QUBO and Ising forms.

```python
from qubovert import boolean_var
from dwave.samplers import SimulatedAnnealingSampler

A, B, C, D, E, F  = boolean_var('A'), boolean_var('B'),
↪  boolean_var('C'), boolean_var('D'), boolean_var('E'),
↪  boolean_var('F')

model = A + B + C + D + E + F
model.add_constraint_OR(A, C, lam=2)
model.add_constraint_OR(A, D, lam=2)
model.add_constraint_OR(A, F, lam=2)
model.add_constraint_OR(B, C, lam=2)
model.add_constraint_OR(B, F, lam=2)
model.add_constraint_OR(D, E, lam=2)
model.add_constraint_OR(E, F, lam=2)

qubo = model.to_qubo()
dwave_qubo = qubo.Q

sampler = SimulatedAnnealingSampler()
result = sampler.sample_qubo(dwave_qubo, num_reads=10)
```

Listing 7: Rewriting MVC with qubovert

---

[3] https://qubovert.readthedocs.io/en/latest/index.html

Listing 7 shows a possible implementation of the MVC problem using the tools provided by qubovert. Qubovert allows us to express our problem as a PCBO; we use this formulation to express constraints in a more natural way. In our example we ensure that each edge is covered simply by enforcing that at least one of the nodes linked by the edge is present in the solution. This constraint is repeated for each edge in the graph (lines 7–13). To specify the Lagrange multiplier (equation **??**) we use the keyword `lam`.

Qubovert, like PyQUBO, can interface with the Ocean SDK, transforming a PCBO problem into a QUBO problem (line 15) and then rewriting it in the format accepted by the D-Wave solver (or sampler).

5.5 CONCLUSION

In this chapter we have set up an environment to run our future experiments and tests. We have also shown some small examples to present the main characteristics and test the tools we will use in our work.

Following this setup allows anyone to recreate exactly the same configuration we use, avoiding (for what we know and test) incompatibilities between Python packages.

6

QA-PROLOG

6.1 THE PROJECT

6.2 PIPELINE

6.3 UPDATE TO THE PROJECT

6.4 RELATED WORK

6.5 CONCLUSION

Part III

EXPERIMENTS

7 A QUANTUM ONTOLOGY

7.1 ONTOLOGY STRUCTURE

7.2 PROLOG VERSION

7.3 INFERENCE ON THE ONTOLOGY

7.4 CONCLUSION

8 QAOA

8.1 QAOA

8.2 FROM QUBO TO PAULI OPERATOR

8.3 EXPERIMENTS

8.4 CONCLUSION

9 CONCLUSION

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