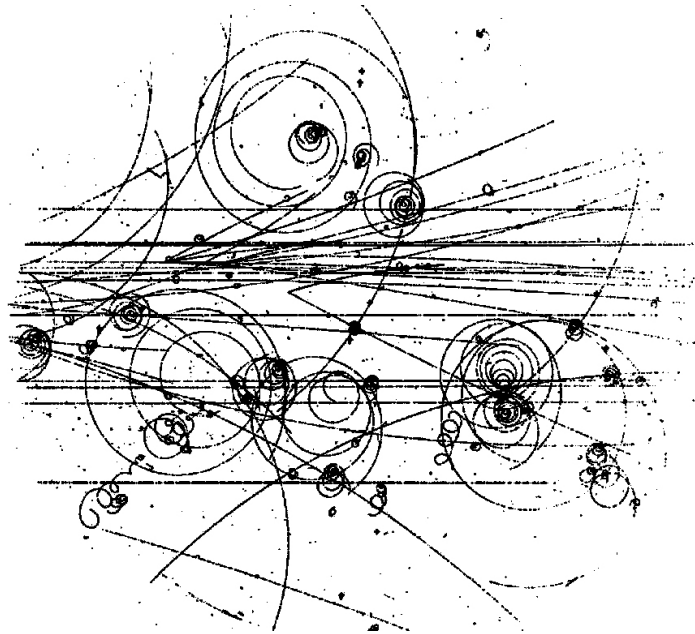


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# QUANTUM COMPUTING FOR LOGICAL INFERENCE

Subtitle





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## Part I

### THEORETICAL BASES



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 measurements

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  $\theta$  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  $\sigma_x$ . 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  $\theta$  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  $\langle \sigma_n \rangle = \hat{n} \cdot \hat{n}^3$ .

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 experiments

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  $\sigma_x$  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

<sup>1</sup> A versor is a vector of magnitude 1 (unit vector), it is normally used to specify a direction.

<sup>2</sup> We can use directly the angle because we are considering versors.

<sup>3</sup> The Dirac bracket  $\langle \rangle$  denotes the statistical mean of a quantity. We call that expectation value.



82 result, the initial configuration (with  $\sigma_z = +1$ ) is lost forever, the only result  
83 we can predict is that  $\langle \sigma_z \rangle = 0$ .

#### 84 1.1.2 Qubit

85 We have introduced the spin referring to electrons in a magnetic field. How-  
86 ever, we can study the spin without examining the associated electron; we  
87 have isolated a simple physical system, the simplest we can study.

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

#### 92 1.1.3 Boolean Logic

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

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

- 101 • The extracted ball is red.
- 102 • The number on the extracted ball is even.

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

- 108 • The extracted ball is red *or* even.
- 109 • The extracted ball is red *and* even.

110 Again it is simple to associate a truth value to these propositions if we con-  
111 sider a single state; also we can construct two subsets that satisfy the propo-  
112 sitions from the subsets we defined before: the new subsets are respectively  
113 the union and intersection of the old ones.

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

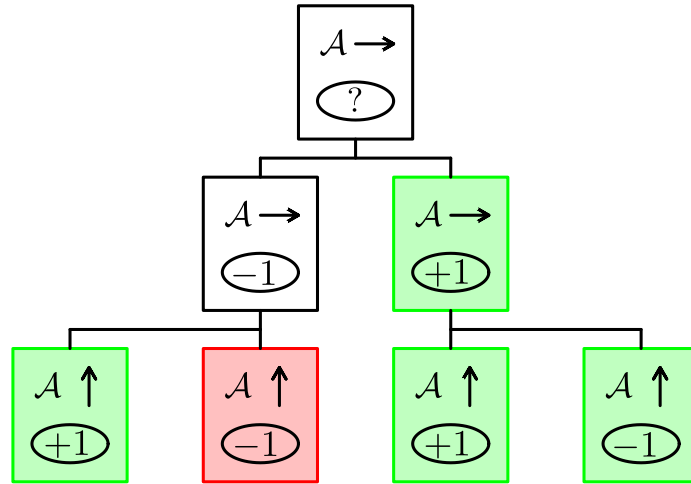
- 116 • The  $z$  component of the spin is  $+1$ .
- 117 • The  $x$  component of the spin is  $+1$ .

118 If we want to check the first proposition we can orient the apparatus  $\mathcal{A}$  along  
119  $z$  and make a measurement; the same procedure can be followed for the  
120 second proposition. The disjunction and conjunction of these propositions  
121 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  $+1$ .

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  $\sigma_z$  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.

The disjunction is not commutative.



**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 which we can immediately conclude that the disjunction of the propositions is true

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.

The conjunction loses its meaning.

## 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.

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: *Hilbert space*

- 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  $\alpha_1$  and  $\alpha_2$  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  $|A\rangle$ :

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

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: *Inner product*

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

Having the inner product we can define:

**VECTOR** 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  $\mathcal{B} = \{|i_1\rangle, |i_2\rangle, \dots, |i_N\rangle\}$  of a space with N dimensions, we can write a generic vector in that space as

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

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

$$\alpha_i = \langle i | A \rangle. \quad (1.2)$$

### 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<sup>4</sup>. 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

<sup>4</sup> We remember that a measure along one axis destroys our knowledge about the result along another axis.

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.

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*  $|o\rangle$ .

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.

*Spin space states have two dimensions*

To express a vector we need a basis; we choose  $\mathcal{B} = \{|u\rangle, |d\rangle\}$ <sup>5</sup> 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  $\alpha_u$  and  $\alpha_d$  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).

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

*Probability amplitudes*

$$\begin{aligned} P_u &= \langle A|u\rangle \langle u|A\rangle \\ P_d &= \langle A|d\rangle \langle d|A\rangle. \end{aligned} \quad (1.3)$$

Components  $\alpha_u$  and  $\alpha_d$  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

<sup>5</sup> We will show that these vectors are in fact orthogonal and why they need to be.

<sup>6</sup> 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.

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.

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  $\mathcal{B} = \{|u\rangle, |d\rangle\}$ . The representation of the basis vectors themselves is naturally easy:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (1.4)$$

$$|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.5)$$

To construct vector *right*, let's consider a spin prepared in the state  $|r\rangle$ . If we measure  $\sigma_z$ , 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:

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

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:

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

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:

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

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

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<sup>7</sup>.

<sup>7</sup> 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* ( $\mathbf{M}$ ) 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<sup>8</sup>.

### 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:

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

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  $\lambda$  the eigenvalue.

*Eigenvalues and eigenvectors*

<sup>8</sup> The reason why we need this kind of operator will be clear in 1.3.2.

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

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

313 We can now write:

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

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

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

316 Hermitian operators have some important properties:

- 317 • all eigenvalues are real;
- 318 • eigenvectors form a *complete set*: all vectors obtained with the applica-  
 319 tion of the operator can be expressed as a linear combination of eigen-  
 320 vectors;
- 321 • if  $\lambda_1$  and  $\lambda_2$  are different eigenvalues, the associated eigenvectors are  
 322 orthogonal;
- 323 • if two eigenvalues are equal (*degeneracy*), it is always possible to find  
 324 two associated eigenvectors that are orthogonal.

Fundamental theorem 325 The last three properties can be summed up in the following way:

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

### 327 1.3.2 Principles of quantum mechanics

328 Let's introduce the first four principles of quantum mechanics, the ones  
 329 about observables<sup>9</sup>.

330 **Principles 1.** *Observables in quantum mechanics are described by linear operators*  
 331  **$\mathbf{L}$ .**

332  $\mathbf{L}$  must also be a Hermitian operator: we can consider this proposition an  
 333 axiom itself or deduce it from the other principles.

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

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

---

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



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

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

347 The inner product is a measure of how much two states are indistinguish- *Overlap*  
 348 able; for that reason it is also called overlap. Two states are physically dis-  
 349 tinct if the overlap is zero.

$$\begin{aligned}\langle u | d \rangle &= 0 \\ \langle u | r \rangle &\neq 0\end{aligned}$$

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

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

352 where  $\lambda_i$  is a generic eigenvalue of  $L$  and  $\langle \lambda_i |$ ,  $|\lambda_i\rangle$  are the bra and ket asso-  
 353 ciated with that eigenvalue (eigenvector of  $\lambda_i$ ).

### 354 1.3.3 Spin Operator

355 The principles tell us what properties a machine must have to represent an  
 356 observable. Let's construct the spin operator  $\sigma$ .

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

362 **OPERATOR  $\sigma_z$ :** Let's start with the simplest operator<sup>10</sup>. The second prin-  
 363 ciple says that all eigenvectors of  $\sigma_z$  are  $|u\rangle$  and  $|d\rangle$ , with associated eigen-  
 364 values  $+1$  and  $-1$ . We can write this assertion as equations:

$$\begin{aligned}\sigma_z |u\rangle &= |u\rangle \\ \sigma_z |d\rangle &= -|d\rangle .\end{aligned}$$

365 In matrix form:

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

366 The solution of this system is<sup>11</sup>:

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

<sup>10</sup> This is because we have chosen  $\mathcal{B} = \{|u\rangle, |d\rangle\}$  as the basis.

<sup>11</sup> It is easy to verify that this operator is also linear.

**OPERATOR  $\sigma_x$ :** 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  $\sigma_x$  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  $\sigma_y$ :** 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:

$$\begin{aligned} \sigma_y |i\rangle &= |i\rangle \\ \sigma_y |o\rangle &= -|o\rangle. \end{aligned}$$

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  $\sigma_z$ ,  $\sigma_x$ , and  $\sigma_y$ :

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (1.10)$$

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

#### 1.3.4 Theory and experiments

Thanks to the operators  $\sigma_z$ ,  $\sigma_x$ , and  $\sigma_y$ , 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  $\sigma$  behaves as a 3-vector, in order to obtain  $\sigma_n$  we only need the inner product:

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

Expanding the components:

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

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

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

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

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

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

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

397 and

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

398 It should be pointed out that the theory is in agreement with experimen-  
 399 tal results<sup>12</sup>. Eigenvalues are  $+1$  and  $-1$ , exactly the only results that the  
 400 apparatus  $\mathcal{A}$  can retrieve. The probability of obtaining a certain result can  
 401 be evaluated as:

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

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

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

*Expectation value*

406 Expected values are obtained as:

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

407 Specifically:

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

408 This is in complete agreement with the experimental results.

409 Before going on, we present, without proof, a useful theorem about expect-  
 410 ation values:

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

$$\langle \mathbf{L} \rangle = \langle A | \mathbf{L} | A \rangle \quad (1.11)$$

413 where  $\mathbf{L}$  is an observable,  $|A\rangle$  is a state vector, and  $\langle A|$  is the corresponding  
 414 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  $\sigma$  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  $|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ . If we apply the operator  $\sigma_z$ , we would obtain again  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ , 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  $\sigma_z$ , 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<sup>13</sup>.

*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

<sup>13</sup> 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.

in quantum mechanics and is called *unitarity*<sup>14</sup>, and it assures us that no information is lost. The unitarity law can be expressed as:

**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:

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

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: *Determinism*

**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:

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

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): *Conservation of Distinctions*

$$\langle \Psi(t) | \Phi(t) \rangle = 0 \quad \forall t \geq 0.$$

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:

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

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.

<sup>14</sup> 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.

In quantum mechanics we can follow the same path and consider time intervals  $\epsilon$  close to zero. In this scenario, after an  $\epsilon$  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:

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

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  $\epsilon \rightarrow 0$ , 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:

$$\hbar \frac{\partial |\Psi\rangle}{\partial t} = -i\mathbf{H}|\Psi\rangle \quad \text{or} \quad \frac{\partial |\Psi\rangle}{\partial t} = \frac{-i\mathbf{H}|\Psi\rangle}{\hbar}. \quad (1.15)$$

*Time-dependent  
Schrödinger equation*

The constant  $\hbar$  has units of  $\text{kg} \cdot \text{m}^2/\text{s}$  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  $\epsilon$ , 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<sup>15</sup> is:

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

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

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

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  $\mathbf{H} \mathbf{L} - \mathbf{L} \mathbf{H}$  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 physics, and the commutator between two operators, in this case  $\mathbf{H}$  and  $\mathbf{L}$ , is denoted by:

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

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

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

or equivalently:

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

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

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

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

### 538 1.4.5 Conservation of Energy

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

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

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

$$[H, H] = 0.$$

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

## 551 1.5 CONCLUSIONS

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

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

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

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

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

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



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

586 All the information that we have learned allows us to understand the con-  
 587 straint of writing only reversible algorithms for quantum-gate-based quan-  
 588 tum computers. Quantum gates operate on qubits through physical transfor-  
 589 mations<sup>17</sup>. These transformations, like all transformations in quantum me-  
 590 chanics, are described by unitary operators that are intrinsically reversible.  
 591 This means that all quantum gates are reversible.

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

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

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

---

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

605



# 3 | QUANTUM ANNEALING

606



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

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

## 616 4.1 KNOWLEDGE BASE

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

### 622 4.1.1 Ontology in philosophy

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

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

### 632 4.1.2 Ontology in computer science

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

639 To address the incompatibility problem between software, databases, and  
640 research groups, ontologies have become an important research topic in com-  
641 puter science where the goal is to define standards for data exchange, infor-  
642 mation 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 neuro-symbolic AI systems[3].

## 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.

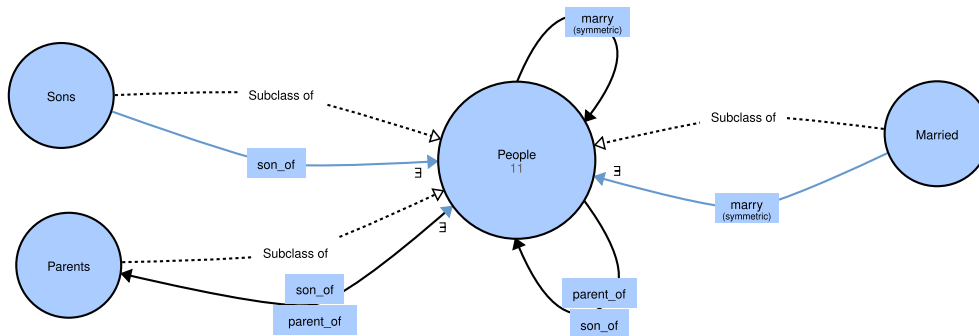


Figure 4.1: Graph for T-Box

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**<sup>1</sup>:

```

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 4.1: 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 (Figure 4.2 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.

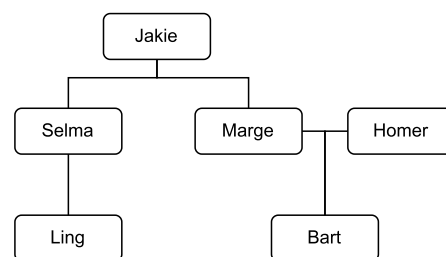


Figure 4.2: Simpson family tree

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.

<sup>1</sup> 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.

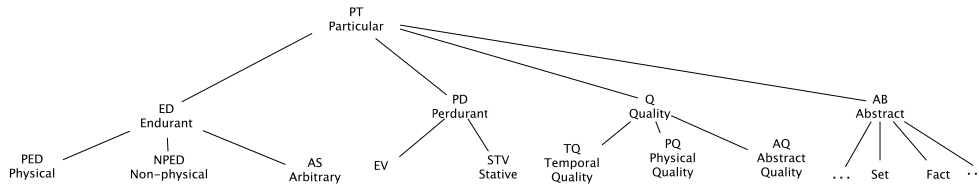


Figure 4.3: First layer of DOLCE taxonomy

**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 REASONING 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 *SROIQ* DL

The semantics of OWL DL extends the semantics of the description logic (DL) *SROIQ* to provide support for datatypes and punning[10]. For con-

777 structs available both in OWL DL and in *SRIOQ* the semantics correspond  
778 exactly.

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

785 *SRIOQ* is one of the most expressive description logics where we have  
786 constructors for:

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

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

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

796 Each of these statements is called an axiom and the set of all axioms consti-  
797 tutes our KB.

#### 798 4.3.2 Interpretation of a knowledge base

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

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

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

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

806 A reasoner should at least be capable of saying if an ontology is consistent,  
807 but we are also interested in querying knowledge to retrieve new informa-  
808 tion.

809 **QUERY INTERPRETATION:** Considering a KB  $K$ , a query  $q$  consists of ax-  
810 iom templates where *SRIOQ* axioms are composed of concept names, role  
811 names, and individual names, but also of concept variables, role variables,  
812 and individual variables. A solution for the query is an interpretation  $\mu$  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  $\mu$  with:[11]

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

In other words  $\mu$  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  $\mu$ , 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.

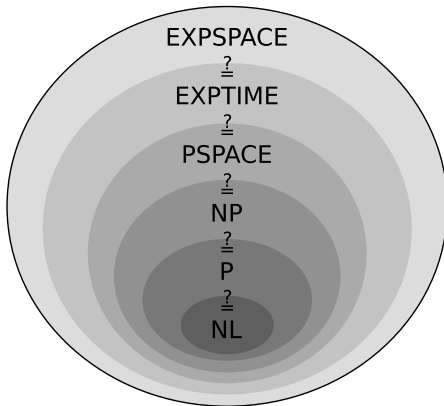


Figure 4.4: Complexity classes

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  $\text{PSpace} = \text{PTime}$ , 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 and evaluates its performance on some real ontologies.

## 858 4.4 CONCLUSIONS

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

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

868

## Part II

869

## TOOLS





870

## 5

## ENVIRONMENT SETUP

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

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

## 876 5.1 PYTHON ENVIRONMENT

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

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

```
882 $ conda create --name quantum python=3.12 pip
$ conda activate quantum
```

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

```
886 $ pip install jupyter
```

## 887 5.2 IBM QISKIT

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

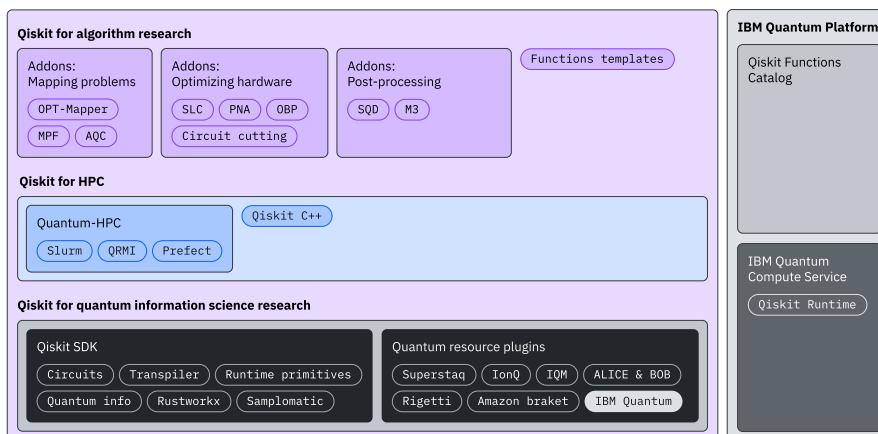


Figure 5.1: Qiskit software stack

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

### 895 5.2.1 Hello World

896 Following the IBM documentation<sup>1</sup> we can install the SDK and the Runtime  
 897 with:

```
898 $ pip install qiskit matplotlib qiskit[visualization]
$ pip install qiskit-ibm-runtime
$ pip install qiskit-aer
```

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

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

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

```
1 from qiskit import QuantumCircuit
2 from qiskit.primitives import StatevectorSampler
3
4 qc = QuantumCircuit(2)
5 qc.h(0)
6 qc.cx(0, 1)
7 qc.measure_all()
8
9 sampler = StatevectorSampler()
10 result = sampler.run([qc], shots=1024).result()
11 print(result[0].data.meas.get_counts())
12 qc.draw("mpl")
```

Listing 5.1: Building Bell state

### 911 5.2.2 Transpilation

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

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

<sup>1</sup> <https://quantum.cloud.ibm.com/docs/en/guides/install-qiskit>

918 topology of a specific QPU. Listing 5.2 implement the transpilation, and  
 919 Figure 5.2 shows the circuits generated: (a) is the circuit we have defined  
 920 in Listing 5.1 and (b) is the transpiled version where the Hadamard gate is  
 921 replaced to match the actual topology of the QPU.

```

1 from qiskit_ibm_runtime.fake_provider import FakeWashingtonV2
2 from qiskit.transpiler import generate_preset_pass_manager
3
4 backend = FakeWashingtonV2()
5 pass_manager = generate_preset_pass_manager(backend=backend)
6
7 transpiled = pass_manager.run(qc)
8 transpiled.draw("mpl")

```

Listing 5.2: Transpilation

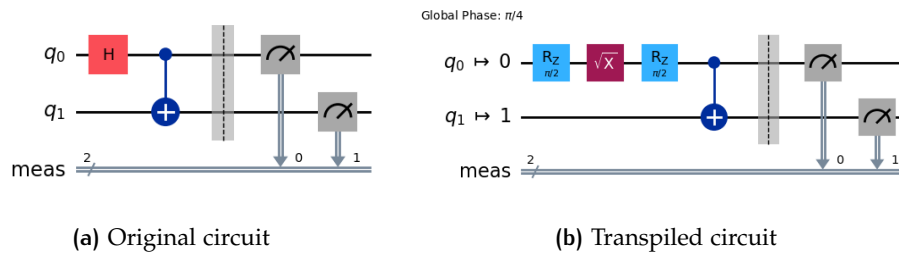


Figure 5.2: Transpilation example

### 922 5.2.3 Execution

923 To test our transpiled circuit we use Aer, which allows us to simulate also  
 924 the noise of real quantum hardware. Listing 5.3 shows how to simulate the  
 execution.

```

1 from qiskit_aer.primitives import SamplerV2
2
3 sampler = SamplerV2.from_backend(backend)
4 job = sampler.run([transpiled], shots=1024)
5 result = job.result()
6 print(f"counts Bell circuit: {result[0].data.meas.get_counts()}")

```

Listing 5.3: Simulated execution

925

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

```

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

```

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

### 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.

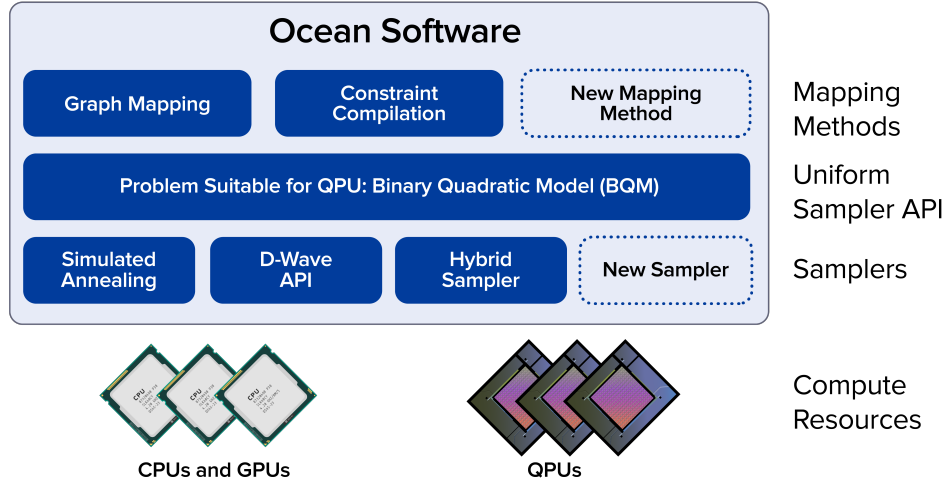


Figure 5.3: Ocean software stack

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

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

955 where  $v$  is the vector containing the binary variables  $v_i$ .

956 The figure shows an example graph (5.4a) and the corresponding matrix  
957 (5.4b) expressing the cost function.

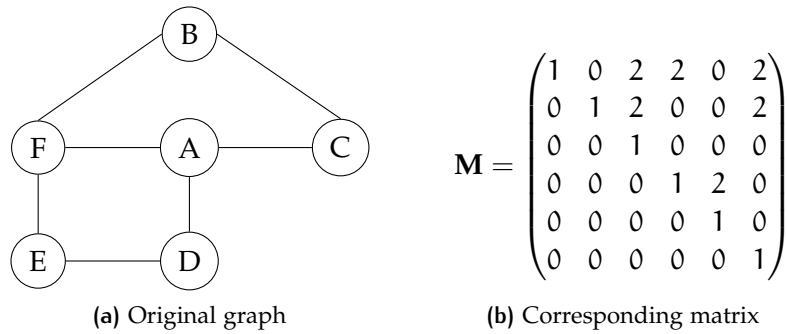


Figure 5.4: Ising formulation

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

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

Listing 5.4: Ising example

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

```
964   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]
```

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

## 967 5.4 PYQUBO AND QUBOVERT

968 In listing 5.4 we have manually built the matrix representing the function  
969 that we want to minimize. It can be useful to have some tools that allow us  
970 to work at a higher level, defining cost functions like ?? that we defined in  
971 the section about quantum annealing (??).

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

### 5.4.1 PyQUBO

Reading from the documentation on the PyQUBO site<sup>2</sup>, 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.

```

1 from pyqubo import Binary, Placeholder, Constraint
2 from dwave.samplers import SimulatedAnnealingSampler
3
4 A, B, C, D, E, F = Binary('A'), Binary('B'), Binary('C'),
5   ↪ Binary('D'), Binary('E'), Binary('F')
6
7 H_objective = (A + B + C + D + E + F)
8 H_penalty = Constraint(((1 - A - C + A*C) + \
9   (1 - A - D + A*D) + \
10  (1 - A - F + A*F) + \
11  (1 - B - C + B*C) + \
12  (1 - B - F + B*F) + \
13  (1 - D - E + D*E) + \
14  (1 - E - F + E*F)), label='cnstr0')
15
16 L = Placeholder('L')
17 H = H_objective + L*H_penalty
18 H_internal = H.compile()
19 bqm = H_internal.to_bqm(feed_dict={'L': 2})
20
21 sampler = SimulatedAnnealingSampler()
22 result = sampler.sample(bqm, num_reads=10)

```

Listing 5.5: Rewriting MVC with pyQUBO

Listing 5.5 presents a possible re-implementation of listing 5.4, 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<sup>3</sup>, 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.

<sup>2</sup> <https://pyqubo.readthedocs.io/en/latest/>

<sup>3</sup> <https://qubovert.readthedocs.io/en/latest/index.html>

Quboververt allows us to define various types of optimization problems that can be solved by brute force, with quboververt's simulated annealing, or with D-Wave's solver. Models defined in quboververt 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, quboververt has a library of famous NP-complete problems mapped to QUBO and Ising forms.

```

1 from quboververt import boolean_var
2 from dwave.samplers import SimulatedAnnealingSampler
3
4 A, B, C, D, E, F = boolean_var('A'), boolean_var('B'),
   ↪ boolean_var('C'), boolean_var('D'), boolean_var('E'),
   ↪ boolean_var('F')
5
6 model = A + B + C + D + E + F
7 model.add_constraint_OR(A, C, lam=2)
8 model.add_constraint_OR(A, D, lam=2)
9 model.add_constraint_OR(A, F, lam=2)
10 model.add_constraint_OR(B, C, lam=2)
11 model.add_constraint_OR(B, F, lam=2)
12 model.add_constraint_OR(D, E, lam=2)
13 model.add_constraint_OR(E, F, lam=2)
14
15 qubo = model.to_qubo()
16 dwave_qubo = qubo.Q
17
18 sampler = SimulatedAnnealingSampler()
19 result = sampler.sample_qubo(dwave_qubo, num_reads=10)

```

Listing 5.6: Rewriting MVC with quboververt

Listing 5.6 shows a possible implementation of the MVC problem using the tools provided by quboververt. Quboververt 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`.

Quboververt, 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).

## 1017 5.5 CONCLUSION

1018 In this chapter we have set up an environment to run our future experiments  
1019 and tests. We have also shown some small examples to present the main  
1020 characteristics and test the tools we will use in our work.

1021 Following this setup allows anyone to recreate exactly the same configura-  
1022 tion we use, avoiding (for what we know and test) incompatibilities between  
1023 Python packages.



1025 QA-Prolog is a tool that allows one to write a program in a logic program-  
 1026 ming language and execute it on a quantum annealer. QA-Prolog also re-  
 1027 trieves the results returned by the quantum annealer and presents them in a  
 1028 natural and comprehensible way.

1029 In this chapter we introduce the project and give some pointers to other  
 1030 related works. We describe extensively the pipeline of transformations that  
 1031 starts from a Prolog code and ends with a Hamiltonian  $H_f$ , as we have  
 1032 described in ?? Next we discuss the changes we have made to the original  
 1033 QA-Prolog code to restore compatibility with the modern framework used  
 1034 to interface with the D-Wave quantum annealer and to support the latest  
 1035 version of the library used in the project.

1036 The chapter ends with an installation guide that ensures a working and  
 1037 reproducible environment to run experiments, both for this chapter and for  
 1038 the following ones.

## 1039 6.1 THE PROJECT

1040 QA-Prolog is a project developed by Scott Pakin<sup>1</sup> in 2017 – 2019. It starts  
 1041 from the question: “Can one express constraint logic programming in the  
 1042 form accepted by quantum-annealing hardware?”[14].

1043 The hope is that even if today we live in the NISQ<sup>2</sup> era of quantum comput-  
 1044 ing, quantum annealers are more easily scalable than quantum gate-based  
 1045 computers[15], and QA-Prolog could improve Prolog program execution by  
 1046 replacing backtracking with fully parallel annealing into a solution state[16].

### 1047 6.1.1 Reason

1048 As we have shown in ?? and ??, programming a quantum computer is not  
 1049 an easy task. We express our algorithm in a very low-level way.

1050 On a quantum annealer we have to define a cost function, without con-  
 1051 straints (which must be transformed into a penalty function). Even if there  
 1052 are libraries that allow us to express these functions in an easier way, we  
 1053 need at least to find a QUBO representation of our problem.

1054 Even worse is the situation on quantum gate-based computers. The pro-  
 1055 grammer has to build a quantum circuit gate by gate, an approach similar  
 1056 to what is done with FPGAs (Field Programmable Gate Arrays)[17]. We can  
 1057 indeed see a strong analogy:

<sup>1</sup> Los Alamos National Laboratory: [pakin@lanl.gov](mailto:pakin@lanl.gov).

<sup>2</sup> Noisy intermediate-scale quantum computing.

- 1058 • programmable logic blocks which implement logic functions → quan-  
1059 tum gates;
- 1060 • programmable routing that connects these logic functions → the possi-  
1061 bility to define the order of gates;
- 1062 • I/O blocks connected to logic → input *qubits* and output *qubits* that we  
1063 can measure.

1064 FPGAs are components that the majority of computer scientists are not used  
1065 to and are probably out of the interest of a programmer. In the same way,  
1066 the hardness of programming a quantum computer could be a significant  
1067 deterrent to attracting new researchers in the field.

1068 In conclusion, even if there exist some sort of abstractions with “high-  
1069 level gates” that wrap multiple low-level gates into useful patterns and there  
1070 exist, both for quantum gate-based computers and quantum annealers, some  
1071 templates of well-known problems that need only fine-tuning to be useful  
1072 for a specific problem, programming a quantum computer is, today, very  
1073 close to machine language.

1074 The goal of QA-Prolog is to fill the gap between the high-level descrip-  
1075 tion provided by a powerful logic programming language and promising  
1076 quantum computers.

### 1077 6.1.2 Prolog

1078 We can see QA-Prolog as a compiler from Prolog to  $H_f$ , where the ground  
1079 state of  $H_f$  is the solution of our Prolog program. Before starting with the  
1080 compilation process, it is useful to understand the main characteristics of  
1081 Prolog, because it is not an imperative programming language like C or  
1082 Java, but a declarative one. For more information about Prolog, the lectures  
1083 of [18] and [19] are recommended.

1084 In Prolog we do not specify step by step an algorithm that resolves our  
1085 problem; instead we describe the formal relationship between the objects in  
1086 our problem and which relations have to be true in our solution[18].

1087 Programming in Prolog consists of:

- 1088 • listing *facts* about objects and relationships between objects;
- 1089 • specifying *rules* to derive new facts from the ones already asserted;
- 1090 • asking questions (*queries*) about objects and their relationships.

1091 From these characteristics we can understand what “declarative” means:  
1092 the program is a list of statements about our problem (our domain of inter-  
1093 est); the relation between a Prolog program and an ontology is very strict.  
1094 In Prolog we encode a knowledge base made of facts and rules; in ?? we can  
1095 see a complete example of rewriting from an OWL ontology into a Prolog  
1096 KB. Moreover, Prolog is a logic programming language. This means that  
1097 the core of programming is not to tell the computer what to do, but to tell  
1098 it what is true and ask it to try to draw conclusions[18]. The idea behind  
1099 logic programming is very interesting; for more details [20] and [21] are  
1100 recommended.

1101 **EXAMPLE:** In the following listing, adapted from [19], we present a basic Prolog program in order to show the syntax and the usage of queries.

```

1 sings(mia).
2 listens2Music(yolanda).
3 party.
4
5 dance(yolanda):- listens2Music(yolanda).
6 happy(yolanda):- dance(yolanda).
7 happy(mia):- sings(mia).
8
9 smile(X) :- happy(X).
```

Listing 6.1: text

1102  
1103 The first three lines are facts; we are asserting that Yolanda is listening to  
1104 music, Mia is singing, and there is a party. The other lines are rules; we can  
1105 identify rules by the `:-` sign that divides the *head* of the rule, on the left, from  
1106 the *body* on the right. The head of a rule is true if the body is true.

1107 For example, the rule at line seven can be read as: “If Mia is singing, then  
1108 Mia is happy”. Line nine shows the usage of a variable; variables start with  
1109 an uppercase letter and are placeholders for information. We can read this  
1110 rule as “If someone is happy, he smiles”.

1111 We can query our KB, asking for example if Yolanda is happy. In SWI-  
1112 Prolog[22] we can interact with the interpreter, and the query we evaluate is:  
1113 `?- happy(yolanda).` (the full stop is part of the syntax and tells the interpreter  
1114 that the query is complete). Prolog will answer `yes.`; this is because Yolanda  
1115 is listening to music, and if she is listening to music she dances, and if she  
1116 dances she is happy.

1117 By analogous reasoning it should be clear why the result of `?- smile(X).`  
1118 is `X = mia; X = yolanda.`, where `;` means logical disjunction: *or*.

### 1119 6.1.3 Feature of QA-Prolog

1120 QA-Prolog does not support all the features of Prolog, but enough to make  
1121 basic logic programming possible[14].

1122 QA-Prolog supports atoms and positive integers but not floating-point  
1123 numbers, strings, or lists. It supports arithmetic and relational operations,  
1124 and rules can reference other rules but not recursively. QA-Prolog supports  
1125 unification, backtracking, and predicates comprising multiple clauses[14].

1126 QA-Prolog also supports some features not present in the basic version  
1127 of Prolog. In particular, operations can be performed on variables even be-  
1128 fore they are ground[14]; this means that QA-Prolog is more powerful in  
1129 manipulating free variables.

### 1130 6.1.4 Related works

1131 There are some other attempts to develop a high-level programming lan-  
1132 guage for quantum computers, both for the quantum gate model and for  
1133 quantum annealers.

1134 *Quantum Prolog* [23] demonstrates that one can express the equivalent of  
 1135 a pure version of Prolog over finite relations in terms of a model of dis-  
 1136 crete quantum computing. This work targets quantum gate computers and  
 1137 focuses on the mathematical equivalence of relational programming and dis-  
 1138 crete quantum computing over the field of Booleans [14].

1139 *C to D-Wave* [24] reuses the pipeline we will discuss, replacing the starting  
 1140 step: the paper addresses the difficulty of programming quantum annealers  
 1141 by presenting a compilation framework that compiles a subset of C code into  
 1142 quantum machine instructions to be executed on a quantum annealer.

## 1143 6.2 PIPELINE

1144 We are now ready to describe the pipeline of transformations that brings us  
 1145 from a Prolog program to a Hamiltonian  $H_f$ .

1146 The chain of transformations is shown in Figure 6.1, where the last step (in  
 1147 orange) is the quantum annealer capable of finding the ground state of  $H_f$ .  
 1148 In purple we can see the various file formats throughout the pipeline, and  
 1149 in yellow the software that performs the rewriting. Some of this software  
 1150 is made ad hoc for the QA-Prolog pipeline; others are also used in very  
 1151 different fields.

1152 From a high-level point of view, the  
 1153 pipeline rewrites the initial knowledge base  
 1154 expressed in Prolog into different objects.  
 1155 The logical meaning of the entities we build  
 1156 during the pipeline is:

- 1157 1. Prolog program (KB);
- 1158 2. High-level digital circuit in Verilog;
- 1159 3. Low-level digital circuit in EDIF;
- 1160 4. Symbolic Hamiltonian;
- 1161 5. Physical Hamiltonian.

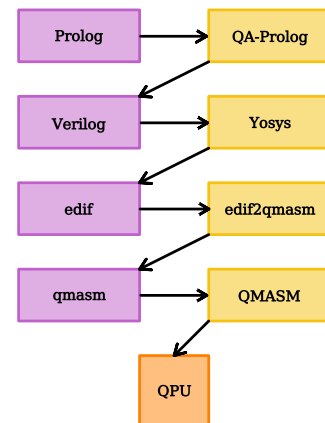


Figure 6.1: QA-Prolog pipeline

1162 Let us start analyzing the pipeline from the last step, the one nearest to the  
 1163 QPU.

### 1164 6.2.1 QMASM

1165 QMASM is a quantum macro assembler[25]; it processes a symbolic Hamil-  
 1166 tonian and assembles a physical Hamiltonian that can be immediately em-  
 1167 bedded on a D-Wave quantum annealer. It was developed by Scott Pakin  
 1168 with the goal of filling a gap in tools for the creation of D-Wave programs.  
 1169 QMASM is an abstraction layer that allows the programmer not to care about  
 1170 manually setting specific point weights and coupler strengths on the physi-  
 1171 cal topology.

This software can be considered an assembler in the sense that it maps a symbolic representation of the operations (assembly language) to the machine language. QMASM is not only an assembler, but extends its functionality by including macros: named blocks of assembly language, parameterized, that a program can instantiate multiple times[25].

**FEATURE:** QMASM provides a number of features to simplify low-level D-Wave programming[25]. Moreover, we can also use QMASM to assemble a physical Hamiltonian that we can later manipulate or solve using classical methods or other quantum systems.

Some of the most useful and interesting features of QMASM are:

- *qubits* are referenced symbolically, not numerically, both in the source code and when QMASM reports execution results;
- *qubits* can be pinned to `true` or `false`;
- *qubit* patterns can be encapsulated into macros and instantiated repeatedly;
- groups of macros can be encapsulated into libraries and reused across multiple programs;
- QMASM can automatically exclude from the results the solutions known to be incorrect and shows only “interesting” *qubits*;

Thanks to this set of features, QMASM is already a useful abstraction layer that simplifies the development of programs that target an annealer, classical or quantum.

**EXAMPLE:** Let us consider an example that shows the potential of QMASM and that is also useful for the following steps of the pipeline. The satisfiability problem is well known to be an NP-complete problem[bibid], so it is a good candidate for our example. We take into account the simple formula:

$$y = x_1 \wedge \neg(x_2 \vee x_3) \quad (6.1)$$

```
# Y = A AND B
!begin_macro AND
  !assert $Y=$A&$B
  $A -0.5
  $B -0.5
  $Y 1

  $A $B 0.5
  $A $Y -1
  $B $Y -1
!end_macro AND
```

(a) *and* gate

```
# Y = NOT A
!begin_macro NOT
  !assert $Y=!$A
  $A $Y 1.0
!end_macro NOT
```

(b) *not* gate

```
# Y = A OR B
!begin_macro OR
  !assert $Y=$A|$B
  $A 0.5
  $B 0.5
  $Y -1

  $A $B 0.5
  $A $Y -1
  $B $Y -1
!end_macro OR
```

(c) *or* gate

Listing 6.2: Logical operators

QMASM allows us to define a macro for every logical operator needed to represent the formula and then assemble the final formula by calling these macros. In Listings 6.2 we call **A** and **B** the input *qubits* and **Y** the output *qubit*. Weights are specified as an Ising problem **??**, which is the default format for QMASM source files<sup>3</sup>.

There are multiple interesting details about these macros:

- the sign **#** tells QMASM that the following line is a comment and should not be processed;
- the sign **\$** is used to tag a *qubit* as ancillary; this means that, unless explicitly requested by the programmer, the intermediate results are not reported in the solutions;
- compared with what we have done in listing 5.4, defining weights is much easier and the result is more readable;
- thanks to the directive **!assert** we can inform QMASM about constraints on the solution; this directive does not change the weights, but allows the programmer to exclude from the solutions those that are surely incorrect.

It is possible to verify, for each macro in listings 6.2, that given a configuration of the input *qubits*, the value of **Y** that minimizes the energy corresponds to the output of the logic gate we are modeling.

We can save these macros in a file named **gates.qasm** and use it to solve our problem. To compute the formula  $y = x_1 \wedge \neg(x_2 \vee x_3)$  we will use some intermediate results: we start with  $x_4 = (x_2 \vee x_3)$ , then we apply the negation  $x_5 = \neg x_4$ , and lastly we compute the result as  $y = x_1 \wedge x_5$ . The QMASM code implementing this procedure is reported in Listing 6.3.

```

1  # Solve circuit-satisfiability problem.
2
3  !include <gates>
4
5  !use_macro OR x2_or_x3
6      x2_or_x3.$A = x2
7      x2_or_x3.$B = x3
8      x2_or_x3.$Y = $x4
9
10 !use_macro NOT not_x4
11     not_x4.$A = $x4
12     not_x4.$Y = $x5
13
14 !use_macro AND x1_and_x5
15     x1_and_x5.$A = x1
16     x1_and_x5.$B = $x5
17     x1_and_x5.$Y = y

```

Listing 6.3: Circuit satisfiability

This example shows how to use macros: we instantiate a macro and give it a name with **!use\_macro <macro\_name> <instance\_name>** (e.g., line five), and

<sup>3</sup> as specified in <https://github.com/lanl/qasm/wiki/File-format>

1225 then instantiate the *qubits* defined in the macro with our actual *qubits*. For  
 1226 example, considering the `!use_macro OR` at line five, we can see that we use  
 1227  $x_2$  and  $x_3$  as input and an ancillary *qubit*  $x_4$  as output. Another detail to  
 1228 point out is the directive `!include` (line three), which imports all gates used  
 1229 in this source file.

1230 Finally, we can query the quantum annealer (or in this case a classical  
 1231 solver) to find a solution for our satisfiability problem. To do so we pin the  
 1232 output variable  $y$  to be sure that in the solution its value will be `true`. We  
 1233 can query the solver with:

```
qasm --run --pin="y := true" --solver="sim_anneal" circ_sat.qasm
```

1234 where `circ_sat.qasm` is the file name of our source code.

1235 Results are reported in listing 6.4. Here we can see that the solver has cor-  
 1236 rectly found the solution, but only 642 times out of the default 1000 samples.  
 1237 This is caused by the stochastic nature of annealing, simulated or quantum;  
 1238 QMASM automatically removed the solutions that do not respect the `!assert`  
 1239 directive or do not have the minimum energy.

```
# x1 --> 12
# x2 --> 3
# x3 --> 4
# y --> [True]
Solution #1 (energy = -20.0000, tally = 642):

Variable  Value
-----  -
x1        True
x2        False
x3        False
y         True
```

Listing 6.4: Circuit satisfiability results

1240 QMASM already offers some powerful abstractions to work with quantum  
 1241 annealers; now we add two additional layers that allow a programming  
 1242 style more similar to the paradigms computer scientists are used to, while  
 1243 preserving strong control over variable dimensions and therefore over the  
 1244 number of *qubits* used.

### 1245 6.2.2 Yosys and edif2qasm

1246 These steps of the pipeline take as input a Verilog HDL (Hardware Descrip-  
 1247 tion Language) program and transform it into a symbolic Hamiltonian.

1248 We aggregate two steps because Yosys is not a tool developed for this  
 1249 pipeline and is used mostly to optimize the intermediate results of the trans-  
 1250 formations. Also, Yosys and edif2qasm work on the same logical entity: a  
 1251 digital circuit that, in these steps of the pipeline, is converted into a symbolic  
 1252 Hamiltonian.

1253 Verilog is a hardware description language that offers different levels of  
 1254 design abstraction. The highest level is “behavioural” and uses program-  
 1255 ming constructs such as assignments, conditionals, and while-loops. The  
 1256 lowest level is a connection of gates (netlists) [26].



Hardware description languages are not something that the majority of programmers are familiar with, but they offer some advantages when targeting a quantum annealer [27]:

- they provide precise control over bit widths in order not to waste any *qubit*;
- they can be compiled to a small set of primitives: the gates we can define with QMASM.

In these steps of the pipeline we follow the same procedure used in the design of digital systems: we start using behavioural constructs, then we automatically generate a netlist as the output of synthesisers.

The synthesiser used is Yosys [28], the first free and open-source software for Verilog HDL synthesis, which supports the vast majority of synthesizable Verilog features.

The two most useful features of Yosys are the possibility of specifying a *cell library*, the set of gates used to synthesize the netlist, and the use of the external tool Berkeley ABC [29] (incorporated in Yosys), providing additional code optimizations.

Yosys lowers a Verilog program to an EDIF netlist that uses only a specified set of gates; then `edif2qasm` lowers the netlist into a symbolic Hamiltonian. This Hamiltonian uses a set of macros defining the energy for each type of gate Yosys can use<sup>4</sup>. What we end up with is a symbolic Hamiltonian that can be used as input for QMASM.

**EXAMPLE:** Considering again the simple formula  $y = x_1 \wedge \neg(x_2 \vee x_3)$  (Equation 6.1), in Figure 6.2 we can see in (a) a possible Verilog implementation of the formula, in (b) the netlist Yosys has produced from the Verilog code, and in (c), only for clarification purposes, the corresponding digital circuit implemented with logic gates.

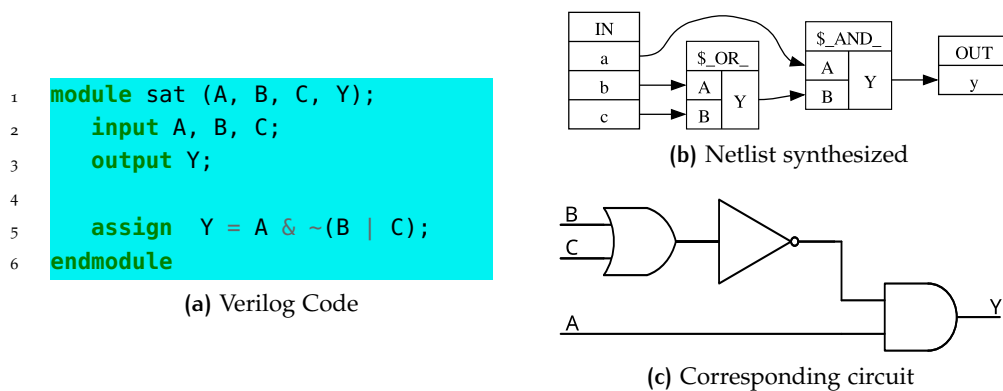


Figure 6.2: Yosys processing

Now we can feed the obtained netlist to `edif2qasm` to obtain the code reported in Listing 6.5.

<sup>4</sup> The actual set of gates extends the logical ports *and*, *or*, and *not* and is available at: <https://github.com/lanl/edif2qasm/blob/master/stdcell.qasm>



```

1  !include <stdcell>
2
3  !begin_macro sat
4      !use_macro AND $id00006
5      !use_macro NOT $id00004
6      !use_macro OR $id00005
7      $id00004.A = $id00005.Y # $or$sat.v:5$1_Y
8      $id00005.A = b
9      $id00005.B = c
10     $id00006.A = a
11     $id00006.B = $id00004.Y # $not$sat.v:5$2_Y
12     $id00006.Y = y
13 !end_macro sat
14
15 !use_macro sat sat

```

Listing 6.5: text

1286 Comparing the automatically generated listing 6.5 and the manually writ-  
 1287 ten 6.3, we can observe some differences:

- 1288 • in listing 6.5 we define the new macro `sat`; this is because each module  
 1289 in the Prolog program is converted into a macro;
- 1290 • the generated code is a little less readable but more compact; we do  
 1291 not need to generate new ancillary variables, but instead use directly  
 1292 as input for macros the output of other macros.

1293 Even if it is less readable, we can comment on the code in 6.5. At lines  
 1294 4, 5, and 6 we declare that we need the macros `AND`, `NOT`, and `OR`, giving to  
 1295 each macro a name like `$id<number>`<sup>5</sup>. At line 7 we assign as input `A` of the  
 1296 macro `NOT` the output `Y` of the macro `OR`. Given these hints, the rest of the  
 1297 code should be clear.

### 1298 6.2.3 QA-Prolog

1299 This is the last step of the pipeline, the one that provides the maximum level  
 1300 of abstraction from the hardware that finds the solution to our problem.

1301 QA-Prolog, like `edif2qasm`, is written in GO[**bibid**] and compiles a Pro-  
 1302 log program to a Verilog one; each fact or rule is converted into a module.  
 1303 Once QA-Prolog has compiled the Prolog source code, including the query  
 1304 that can be specified on the command line, into Verilog, QA-Prolog invokes  
 1305 Yosys, `edif2qasm`, and QMASM, as illustrated in Figure 6.1 [14].

1306 QMASM executes the user's program on a D-Wave system or on a simu-  
 1307 lator and reports the value of each symbol appearing in the QMASM source  
 1308 file. QA-Prolog maps these lists of Booleans back to integers and named  
 1309 atoms, associates those values with variables named in the user's query, and  
 1310 reports all variables and their values to the user just as a typical Prolog en-  
 1311 vironment would [14].

5 the symbol `$` tells QMASM that we are not interested in the value of *qubits* inside the macro

1312 **EXAMPLES:** The first example we present shows a small knowledge base  
 1313 that can be summarized as “the enemy of my enemy is my friend”.

```

1      hates(alice, bob).
2      hates(bob, charlie).
3
4      enemy(A, B) :- hates(A, B).
5      enemy(A, B) :- hates(B, A).
6
7      friend(A, B) :-
8      enemy(A, C),
9      enemy(C, B).
```

Listing 6.6: KB enemy of my enemy is my friend

1314 The code is reported in Listing 6.6. Thanks to the declarative nature of  
 1315 Prolog we can immediately understand the meaning of our KB: we describe  
 1316 relations between three people, assert that if a person hates another one they  
 1317 are enemies (lines 4 and 5), and that if two people share an enemy they are  
 1318 friends (lines 7, 8, and 9).

1319 We can now query the KB to find if there are two people who are friends;  
 1320 we can do that with:

```

QA-Prolog --qmasm-args="--solver=tabu" --query='friends(P1, P2).'
↪ --work-dir=~/.work friends.pl
```

1321 In this command we can see that QA-Prolog allows us to query the KB  
 1322 with the exact same syntax we would use to interact with a Prolog interpreter.  
 1323 As expected, QA-Prolog binds the variables **P1** and **P2** to Alice and Charlie.

1324 Another detail to point out is the parameter `--work-dir=<path>`, which  
 1325 specifies the folder in which QA-Prolog outputs all files, and the solver: we  
 1326 use a tabu search algorithm because the simulated annealing implemented  
 1327 in Ocean is not capable of finding a solution even in this small scenario  
 1328 (more considerations about that in the concluding Chapter ??).

1329 If we inspect the working directory we can see the output of every step  
 1330 of the pipeline; in particular, to see how exactly the KB is rewritten into a  
 1331 Verilog program, in Appendix ?? there is the result of compilation, and it is  
 1332 possible to observe in detail how each fact or rule has been transformed.

1333 The second example concludes our transformation of the satisfiability  
 1334 problem (Equation 6.1); unfortunately, this is not very didactic because the  
 1335 Prolog program suitable for QA-Prolog processing introduces a consistent  
 1336 amount of overhead.

1337 Indeed, we have to implement logical operators by defining their truth  
 1338 tables, then assemble the operators in our logical formula. Listing 6.7 shows  
 1339 the implementation we use in our test.

1340 We can now run QA-Prolog with the query `sat(A, B, C, true)` to find the  
 1341 correct assignment of Boolean variables that satisfy our logic formula. Again,  
 1342 we are forced to use the tabu search algorithm.

```

1  and(false, false, false).
2  and(false, true, false).
3  and(true, false, false).
4  and(true, true, true).
5
6  not(false, true).
7  not(true, false).
8
9  or(false, false, false).
10 or(false, true, true).
11 or(true, false, true).
12 or(true, true, true).
13
14 sat(A, B, C, Y) :-
15   or(B, C, X),
16   not(X, Z),
17   and(A, Z, Y).

```

Listing 6.7: text

#### 1343 6.2.4 Overview

1344 We have described a pipeline of rewritings that, layer after layer, makes it  
 1345 possible to abstract away from the hardware that actually solves our prob-  
 1346 lem, moving toward a language, and thus a way of reasoning, that is at a  
 1347 higher level. We speak of rewritings because the object we are manipulating  
 1348 remains logically unchanged, just as it is essential that the solutions we are  
 1349 searching for remain unchanged; the problem and its solutions are simply  
 1350 expressed in different languages as one moves down the pipeline.

1351 The advantages of abstraction are essentially the same as those obtained  
 1352 when moving from assembly language to a high-level language: greater ease  
 1353 of expression, improved readability, and the possibility of working with al-  
 1354 ready familiar paradigms. The drawbacks are the overheads that naturally  
 1355 arise during the translation process. QA-Prolog is still a prototype, and if to-  
 1356 day compilers produce better machine code than a programmer could write  
 1357 manually, it is because significant effort and many years of research have  
 1358 been invested to achieve excellent results. The hope is that QA-Prolog and  
 1359 related works represent a first step in the same direction within the field of  
 1360 quantum computing.

## 1361 6.3 UPDATE TO THE PROJECT

1362 In this section we briefly describe the updates we have made to the project in  
 1363 order to restore compatibility with the Ocean framework and with the other  
 1364 libraries used. We also provide a small guide to install the tools to ensure  
 1365 that all packages work properly and our experiments are reproducible.

### 1366 6.3.1 Restoring QMASM

1367 The last commit to QA-Prolog was made in 2019, and the last one to QMASM  
1368 in 2021. Since then, packages and libraries have changed and the compati-  
1369 bility with the QA-Prolog pipeline has broken.

1370 The most fragile component of the pipeline is QMASM, because it is the  
1371 one that interacts with external frameworks that are likely to change. In par-  
1372 ticular, the development of Ocean is very active, and some functions used in  
1373 QMASM have now been removed, deprecated, or moved to other packages.

1374 The incompatibilities encountered between imports used in QMASM and  
1375 external libraries are:

- 1376 • in the `dwave.cloud` and `hibrid` libraries;
- 1377 • in the libraries defining D-Wave samplers (classical solvers);
- 1378 • in the `scipy.stats` library.

1379 The documentation available for Ocean<sup>6</sup> and for scipy<sup>7</sup> helped us resolve  
1380 these incompatibilities: most of the time the solution consisted simply in  
1381 correcting the name of the library.

1382 Another small bug, caused by a different name of a solver in the command  
1383 line helper and in the actual code, was fixed by restoring the correspondence.

### 1384 6.3.2 Fixing interaction edif2qasm-QMASM

1385 During the execution of the complete pipeline we encountered an error  
caused by undefined macros in the QMASM source file.

```
1 // Define hates(atom, atom).
2 module \hates/2 (A, B, Valid);
3   ...
4 endmodule
```

(a) Verilog Code

```
1 # hates/2
2 !begin_macro id00011
3   ...
4 !end_macro id00011
```

(b) Macro definitions

```
1 # enemies/2
2 !begin_macro id00010
3   !use_macro hates/2 $id00032 # hates_PWYwG/2
4   ...
5 !end_macro id00010
```

(c) Macro usage

Listing 6.8: text

1386 The error can be seen in Listings 6.8: edif2qasm rewrites the netlist  
1387 generated from (a) into the macro (b); here `hates/2` is just a comment, the  
1388 actual name of the macro is `id00011` (specified at line 2). In (c), however,  
1389 we can see that the macro previously defined is called symbolically and not  
1390 with its actual name (lines 3). This obviously produces an error: the name  
1391 `hates/2` in the QMASM file has no meaning, it is only a comment.

6 available at <https://docs.dwavequantum.com/en/latest/index.html>

7 available at <https://docs.scipy.org/doc/scipy/index.html>

```

1 with open(file, 'r') as input:
2     first = input.readline()
3     second = input.readline()
4     while(second_row != ""):
5         if first.startswith("#") and second.startswith("!begin_macro"):
6             self.name[first[2:-1]] = second[len("!begin_macro "):-1]
7             first_row = second_row
8             second_row = input.readline()
9
10 with open(file, 'r') as input:
11     doc = input.read()
12     lines = doc.splitlines()
13     for line in lines:
14         for word in line.split():
15             if word in self.name.keys():
16                 line = line.replace(word, self.name[word])
17             self.new_lines.append(line)

```

Listing 6.9: text

1393 To solve the problem we added a preprocessing step before parsing with  
 1394 QMASM. During the preprocessing all symbolic names are substituted with  
 1395 the actual name of the corresponding macro.

1396 The core code of the preprocessor is reported in Listing 6.9. The program  
 1397 scans the source file two times: during the first reading a python dictio-  
 1398 nary *symbolic\_name-actual\_name* is built, then, during the second reading, all  
 1399 instances of the symbolic name are replaced with the actual name.

1400 Now all components should work properly, and we can install all the  
 1401 software needed and run some experiments.

### 1402 6.3.3 Installation guide

1403 In order to have a working environment where we can run our experiments  
 1404 we need to install all the software required by the QA-Prolog pipeline. In  
 1405 Chapter 5 we have set up a python environment with all the essential tools;  
 1406 to start the installation of the QA-Prolog pipeline we need at least the Ocean  
 1407 SDK installed as described in 5.3.

1408 The first component we need is QMASM; we can install the updated and  
 1409 fixed version from <https://github.com/DavideCamino/qasm.git>. The in-  
 1410 stallation procedure consists of the following three commands:

```

1 $ git clone https://github.com/DavideCamino/qasm.git
2 $ cd qasm
3 $ python setup.py install

```

1411 Next we need Yosys and GO; Yosys is part of the pipeline, and GO allows  
 1412 us to compile edif2qasm and QA-Prolog. Both Yosys and GO are available  
 1413 as binary packages for the majority of GNU/Linux distributions; on Arch<sup>8</sup>  
 1414 they can be installed with:

---

8 <https://archlinux.org/>

```

1  # pacman -S yosys
2  # pacman -S go

```

The `go install` command installs Go executables in the default directory `$HOME/go/bin`; it is useful to add the bin subdirectory to `PATH`. This can be done by editing the `.bashrc` file (or the corresponding one for the specific shell), adding:

```

1  PATH=$PATH:$HOME/go/bin
2  export PATH

```

Finally we can install `edif2qasm` and `QA-Prolog` with:

```

1  $ go install github.com/lanl/edif2qasm@latest
2  $ go install github.com/lanl/QA-Prolog@latest

```

## 1420 6.4 CONCLUSION

1421 In this chapter, we presented QA-Prolog, a rewriting pipeline that enables  
 1422 the transformation of a Verilog program into a Hamiltonian whose ground  
 1423 state represents the solution of the original program. We discussed the vari-  
 1424 ous steps of the pipeline in detail, also showing how some parts were mod-  
 1425 ified to make them compatible again with current frameworks. Finally, we  
 1426 described how to install a working version of the pipeline.

1427 From our discussion, it emerges that QA-Prolog is a modular software  
 1428 stack in which it is possible to replace a component of the pipeline with  
 1429 another to modify the result; for example, we presented work that starts  
 1430 from C instead of Prolog.

1431 This work has the potential to provide a foundation for many other exper-  
 1432 iments that can rely on an already implemented and functioning infrastruc-  
 1433 ture in order to develop new extensions both upstream and downstream of  
 1434 the pipeline.

Part III

EXPERIMENTS





# 1437 7 | A QUANTUM ONTOLOGY

## 1438 7.1 ONTOLOGY STRUCTURE

## 1439 7.2 PROLOG VERSION

## 1440 7.3 INFERENCE ON THE ONTOLOGY

## 1441 7.4 CONCLUSION



## 1442 8 | QAOA

### 1443 8.1 QAOA

### 1444 8.2 FROM QUBO TO PAULI OPERATOR

### 1445 8.3 EXPERIMENTS

### 1446 8.4 CONCLUSION







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