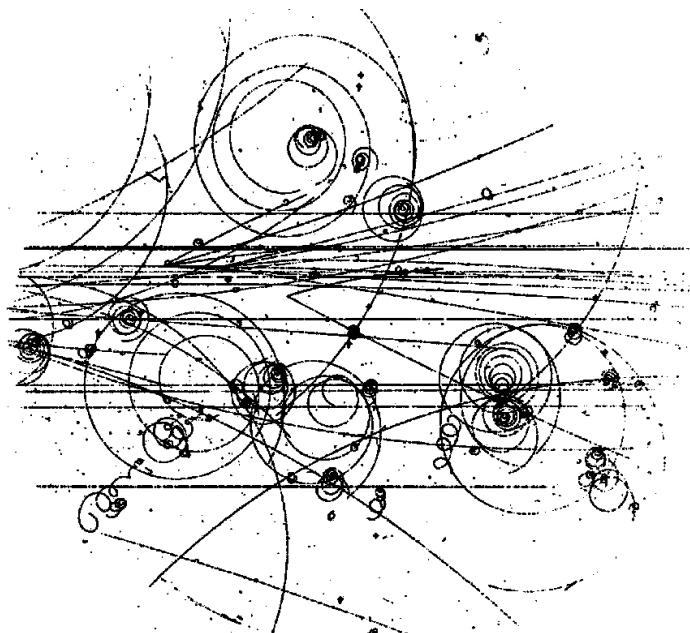


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QUANTUM COMPUTING FOR  
LOGICAL INFERENCE

Subtitle





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Part I  
THEORETICAL BASES



# 1

## QUANTUM MECHANICS

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

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

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

### 1.1 EXPERIMENTS

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

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

#### 1.1.1 Spin

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

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



Figure 1.1: Experiment's schema

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

*Repeatability of measure*  
 42 If we measure the spin of an electron and  $\mathcal{A}$  displays  $+1$ , we can confirm  
 43 the experiment's results by measuring the spin again and we obtain spin  $+1$   
 44 every time. This means that the measurements are repeatable (an essential  
 45 property to construct models and make predictions). We can think, and it  
 46 will be clear later why it is useful, that the first experiment prepares the spin  
 47  $+1$  and the others confirm this result.

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

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

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

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

68 If we start the experiments with a spin prepared as  $\sigma_z = +1$  and then  
 69 orient  $\mathcal{A}$  along a generic axis  $\hat{n}$  each measure would be binary and unpre-  
 70 dictable, but the mean of the measures tends to  $\hat{z} \cdot \hat{n} = \cos \theta$  where  $\theta$  is the  
 71 angle between  $\hat{z}$  and  $\hat{n}$ . In the most general case we can start with the ap-  
 72 paratus oriented like  $m$  and prepare the spin  $\sigma_m = +1$ , then we rotate  $\mathcal{A}$   
 73 around  $\hat{n}$  without interfering with the spin and measure again; we would  
 74 obtain the statistical result  $\langle \sigma_n \rangle = \hat{m} \cdot \hat{n}$ <sup>3</sup>.

75 The result of a single measure is non deterministic, but we can make pre-  
 76 dictions over the mean values of the measures: the expected values behave  
 77 as the single results of the classic experiment.

*Invasive experiments*  
 78 Considering now a sequence of three measures: starting with  $\mathcal{A}$  oriented  
 79 along  $z$  we prepare the spin  $\sigma_z = +1$ , then we rotate  $\mathcal{A}$  to measure  $\sigma_x$   
 80 obtaining, let's say,  $+1$  (the reasoning is the same if we obtain  $-1$ ); lastly  
 81 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:

- 122 • The  $z$  component of the spin is  $+1$  or the  $x$  component is  $+1$ .  
 123 • The  $z$  component of the spin is  $+1$  and the  $x$  component is  $+1$ .

124 Starting with the disjunction. Considering a state prepared, without our  
 125 knowledge, with  $\sigma_z = +1$ . If our first measure is along the  $z$  axis,  $\mathcal{A}$  will  
 126 always display  $+1$  and we can immediately conclude that the proposition  
 127 is true. If we start measuring the  $x$  component, we have a 50% chance that  
 128  $\mathcal{A}$  displays  $+1$  or  $-1$ ; also this measurement destroys the initial state and  
 129 the measure of  $\sigma_z$  becomes non predictable. In this scenario we have a 25%  
 130 chance of deducing that the proposition is false; figure 1.2 shows all the  
 The disjunction is not  
 commutative<sup>g2</sup> possible measurement results in this case. The logical value of a proposition  
 depends on the order in which we perform the measurements.

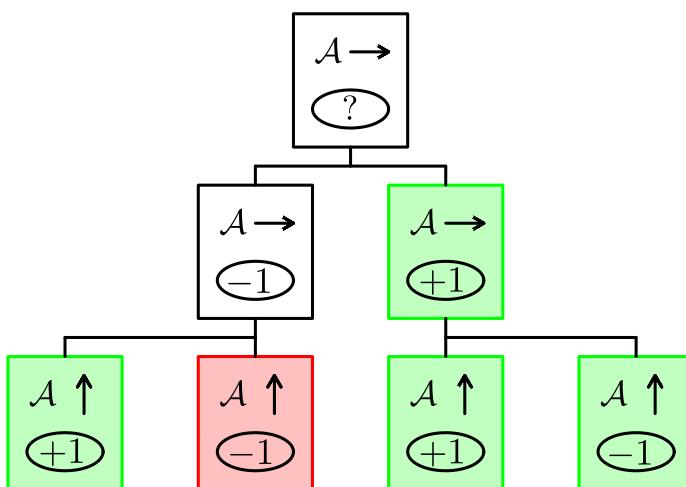


Figure 1.2: The apparatus  $\mathcal{A}$  is represented as a box, the arrow represents the direction along which the apparatus is oriented, the display (ellipse) shows the result of measurement. We have highlighted in green the cases in which we can immediately conclude that the disjunction of the propositions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

133 The conjunction is even worse: no matter the order of the measurements,  
 134 the second one destroys the result of the first. The disjunction is true if at  
 135 least one of the sub-propositions is true, and if we find a spin component  
 136 that is  $+1$  we can always confirm this result with another measurement. In  
 137 the conjunction the two sub-propositions must be true *at the same time*, but  
 The conjunction loses its  
 meaning<sup>g3</sup> with the second measurement we lose all the knowledge of the first one. We  
 can never conclude that the conjunction is true.

## 140 1.2 QUANTUM STATES

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

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

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

147 **1.2.1 Vector Spaces**

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

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

- 155 • the sum of two kets is a ket;
- 156 • addition is commutative;
- 157 • addition is associative;
- 158 • existence of identity element for addition;
- 159 • existence of inverse elements for addition;
- 160 • existence of identity element for scalar multiplication;
- 161 • linearity property.

162 **1.2.2 Bra and Ket**

163 An example of ket that we will find often is the column vector of two dimen-  
 164 sions:

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

165 where  $\alpha_1$  and  $\alpha_2$  are complex numbers. With this simple example of ket it  
 166 is easy to verify the validity of all previously described properties.

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

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

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

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

177 Having the inner product we can define:

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

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

*Inner product*

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.

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  $|\mathcal{A}\rangle$  can be expressed as:

$$|\mathcal{A}\rangle = \alpha_u |u\rangle + \alpha_d |d\rangle$$

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

$|\mathcal{A}\rangle$  components are complex numbers and their physical meaning is: having a spin prepared in the state  $|\mathcal{A}\rangle = \alpha_u |u\rangle + \alpha_d |d\rangle$ <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:

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

*Spin space states have two dimensions*

*Probability amplitudes*

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  $|\mathcal{A}\rangle$  is normalized:  $\langle \mathcal{A} | \mathcal{A} \rangle = 1$ .

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.

252 that if we orient  $\mathcal{A}$  along  $z$  and measure  $\sigma_z = +1 = |\mathbf{u}\rangle$ , we would have  
 253  $\alpha_d = \langle \mathbf{d} | \mathbf{u} \rangle \neq 0$ , which is a contradiction to experimental results. If  $\alpha_d \neq 0$ ,  
 254 then  $\alpha_d^* \alpha_d > 0$ ; we started with a state prepared as  $\sigma_z = +1$  and ended with  
 255 a nonzero probability of measuring  $\sigma_z = -1$ : this is absurd.

*Orthogonal states are mutually exclusive*  
 256 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.

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

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

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

260 To construct vector *right*, let's consider a spin prepared in the state  $|\mathbf{r}\rangle$ . If  
 261 we measure  $\sigma_z$ , we have a 50% chance of obtaining +1 (and 50% for -1); this  
 262 means that for  $|\mathbf{r}\rangle$  we have  $\alpha_u^* \alpha_u = \alpha_d^* \alpha_d = 1/2$ . A vector that satisfies this  
 263 constraint is:

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

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

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

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

- 268 • states must be orthogonal:  $\langle \mathbf{i} | \mathbf{o} \rangle = \langle \mathbf{o} | \mathbf{i} \rangle = 0$ ;
- 269 • if we have a spin prepared as *in* or *out*:
  - 270 – equiprobability of measuring  $\sigma_z = +1$  and  $\sigma_z = -1$ ;
  - 271 – equiprobability of measuring  $\sigma_x = +1$  and  $\sigma_x = -1$ .

272 Two vectors that satisfy these constraints are:

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

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

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

<sup>7</sup> To avoid confusion, we point out that  $|\mathbf{i}\rangle$  is the ket of state *in*. *i*, instead, is the imaginary unit.

## 278 1.3 OBSERVABLES

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

283 In quantum mechanics the situation is more complex; our intuition is mis-  
 284 leading, and we need mathematical tools to describe what we can measure:  
 285 the observables. These tools are mathematical operators called *machines* ( $\mathbf{M}$ )  
 286 and have as both input and output state vectors.

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

288 We will show that machines are Hermitian operators, so let's start defining  
 289 these operators and describing their properties<sup>8</sup>.

## 290 1.3.1 Hermitian operator

291 Formally, machines modify a state vector in this way:

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

292 The linearity of machines implies that:

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

293 and:

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

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

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

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

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

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

*Eigenvalues and eigenvectors*

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

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

---

8 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  $\dagger$ :

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

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 theorems 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.

---

<sup>9</sup> 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 indistin- *Overlap*  
348 guishable; 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.

367 **OPERATOR  $\sigma_x$ :** With the same reasoning, we can construct the operator 368 along the  $x$  axis. We have already deduced the representations of *right* and 369 *left* in equations [1.6](#) and [1.7 on page 10](#). The equations that allow us to 370 construct  $\sigma_x$  are:

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

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

371 The solution of this system is:

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

372 **OPERATOR  $\sigma_y$ :** The last direction is along the  $y$  axis. Considering the 373 expressions for *in* and *out* given in equations [1.8](#) and [1.9 on page 10](#), and 374 following the second principle, we can write:

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

375 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*366 We have obtained a matrix representation of the three spin operators  $\sigma_z$ , 377  $\sigma_x$ , and  $\sigma_y$ :

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

378 These famous and important matrices are named after their inventor, Wolfgang 379 Ernst Pauli.

### 380 1.3.4 Theory and experiments

381 Thanks to the operators  $\sigma_z$ ,  $\sigma_x$ , and  $\sigma_y$ , if we know the state vector, we can 382 statistically predict the result of a measurement of the spin along one of 383 the three coordinate axes. What can we say about a measurement taken by 384 orienting the apparatus  $\mathcal{A}$  along a generic direction?

385 Considering  $\mathcal{A}$  oriented along the unit vector  $\hat{n}$ , if  $\sigma$  behaves as a 3-vector, 386 in order to obtain  $\sigma_n$  we only need the inner product:

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

387 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:

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

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 expec-  
 410 tation 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:*

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

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

---

<sup>12</sup> If not, we must abandon this model and build another one.

415 **1.3.5 Operator and Measure**

416 Operators allow us to know the probability of measuring a certain spin given  
 417 the direction of the measurement and the state vector. This probability is  
 418 expressed by the state vector that we obtain when we apply the operator  $\sigma$   
 419 to the initial state.

420 It is important not to confuse the measurement act with the application  
 421 of a machine that represents the observables. The spin state after the mea-  
 422 surement is not the same as the one we obtain after the application of the  
 423 operator. The operator is only an abstract mathematical construct that allows  
 424 us to make statistical predictions about results, but doesn't have physical im-  
 425 plications.

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

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

- 435 • +1: the final state will be *up*;
- 436 • -1: the final state will be *down*.

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

439 **1.4 TEMPORAL EVOLUTION**

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

442 **1.4.1 Unitarity**

443 In classical mechanics we are used to having a motion law that links differ-  
 444 ent states of our system deterministically; this means being able to know  
 445 precisely the following state given the previous one. A good law, however,  
 446 doesn't allow us only to know the future, but also the past states that brought  
 447 the system to the current state<sup>13</sup>.

Reversibility<sup>13</sup> 448 In other words, we want physical transformations to be reversible. This  
 449 requirement is so important that we call this property the *minus first law*,  
 450 because it underlies everything else. If we think about the system states as  
 451 nodes in an oriented graph, reversibility imposes that each node has exactly  
 452 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.

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

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

457 **1.4.2 Time-Development Operator**

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

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

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

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

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

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

- 467 • be a linear operator;
- 468 • respect reversibility.

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

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

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

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

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

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

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

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

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

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

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

*Conservation of Distinctions*

---

<sup>14</sup> We will see in the next paragraph the reason for this name

## 484 1.4.3 The Hamiltonian

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

*Continuity* 488 In quantum mechanics we can follow the same path and consider time  
 489 intervals  $\epsilon$  close to zero. In this scenario, after an  $\epsilon$  amount of time, the state  
 490 vector will change slightly and “smoothly”, and the operator  $\mathbf{U}(\epsilon)$  will be  
 491 very similar to the identity. We can rewrite  $\mathbf{U}(\epsilon)$  in order to highlight the  
 492 difference with the identity  $\mathbf{I}$  as:

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

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

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

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

497 Bringing to the left the time interval:

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

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

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

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

506 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*

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

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

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

516 Expanding to first order in  $\epsilon$ , we find:

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

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

*Quantum Hamiltonian*

#### 520 1.4.4 Commutators

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

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

524 The time derivative<sup>15</sup> is:

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

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

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

527 That can be rewritten as:

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

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

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

533 With the commutator we can express concisely the derivative of the expec-  
 534 tation value for the observable  $\mathbf{L}$ :

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

535 or equivalently:

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

536 This equation links variations of the expectation values of an observable  
 537 ( $\mathbf{L}$ ) 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  $\mathbf{Q}$ , if  $[\mathbf{Q}, \mathbf{H}] = 0$ , then every power satisfies*  
 545  *$[\mathbf{Q}^n, \mathbf{H}] = 0$ . This means that the expectation value  $\langle \mathbf{Q} \rangle$  is conserved, and any*  
 546 *power of the expectation value  $\langle \mathbf{Q}^n \rangle$  does not change with time.*

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

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

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.

---

<sup>17</sup> How depend strongly on the particular physical implementation.

<sup>18</sup> 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.



605 2 | QUANTUM GATE



606 | 3 QUANTUM ANNEALING



607    **4** | ONTOLOGY

608    **4.1    ONTOLOGY**

609    **4.2    FAMOUS ONTOLOGY**

610    **4.3    RERASONING ON ONTOLOGY**

611    **4.4    CONCLUSION**



612

## Part II

613

## TOOLS



# 5 | ENVIRONMENT SETUP

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

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

## 620 5.1 PYTHON ENVIRONMENT

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

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

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

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

```
1 pip install jupyter
```

## 629 5.2 IBM QISKIT

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

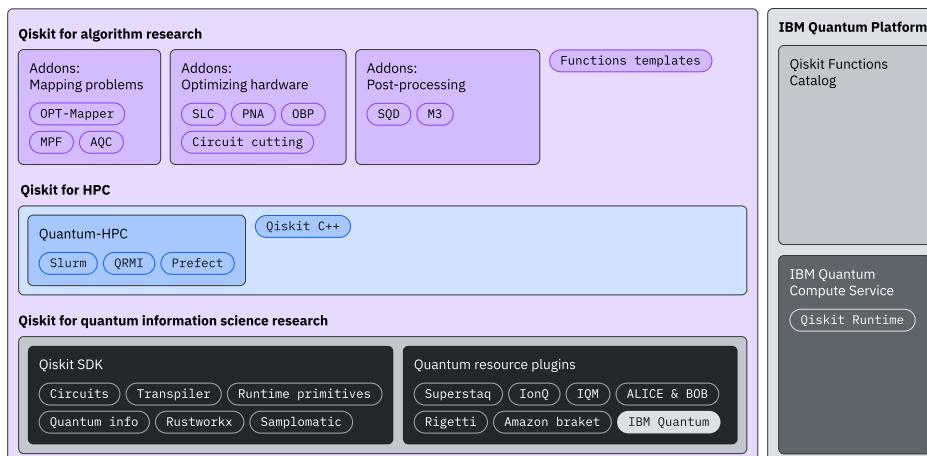


Figure 5.1: Qiskit software stack

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

### 637 5.2.1 Hello World

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

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

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

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

648 If the setup is successful we are now able to run a small test to build a Bell  
 649 state (two entangled qubits). The following code assembles the gates, shows  
 650 the final circuit and uses a sampler to simulate on the CPU the result of 1024  
 651 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 1:** Building Bell state

### 652 5.2.2 Transpilation

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

---

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

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

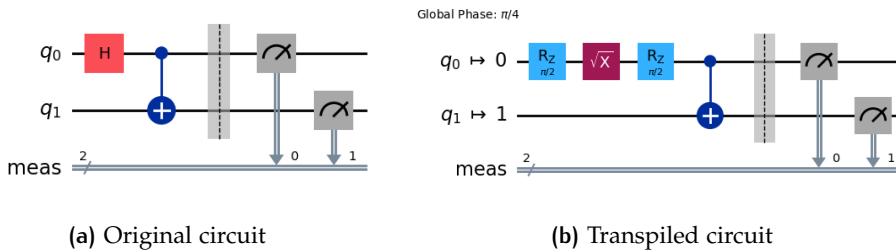
```

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 2:** Transpilation

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



**Figure 5.2:** Transpilation example

662

### 663 5.2.3 Execution

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

```

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 for Bell circuit : {result[0].data.meas.get_counts()}")

```

**Listing 3:** Simulated execution

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

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

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

## 671 5.2.4 A complete example on real hardware

## 672 5.3 D-WAVE OCEAN

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

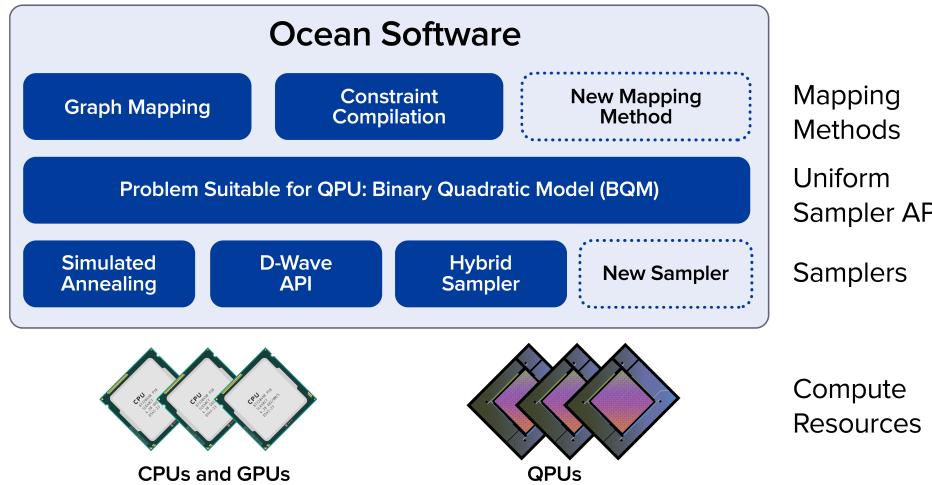


Figure 5.3: Ocean software stack

676  
 677 All tools that implement the steps needed to solve your problem on a CPU,  
 678 a D-Wave quantum computer, or a quantum-classical hybrid solver can be  
 679 installed with:

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

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

## 684 5.3.1 Hello World

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

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

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

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

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

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

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

695 The figure shows an example graph (5.4a) and the corresponding matrix  
 696 (5.4b) expressing the cost function.

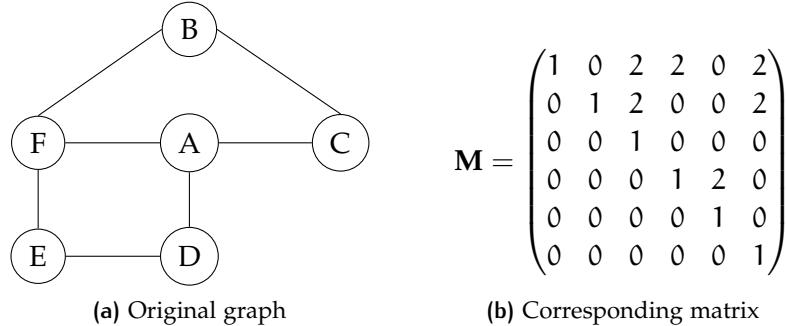


Figure 5.4: Ising formulation

697 The following code presents a possible implementation of the Ising model  
 698 described above. We have defined two dictionaries to store the matrix coeffi-  
 699 cients. The last line of code finds ten possible answers to the problem using  
 700 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 4: Ising example

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

```

1 A B C D E F energy num_oc.
2 0 -1 -1 +1 +1 -1 +1 -14.0 6
3 1 +1 +1 -1 -1 +1 -1 -14.0 4
4 ['SPIN', 2 rows, 10 samples, 6 variables]

```

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

### 705 5.3.2 Example on real hardware

### 706 5.3.3 Minor embedding

## 707 5.4 PYQUBO AND QUBOVERT

708 In listing 4 we have manually built the matrix representing the function that  
 709 we want to minimize. It can be useful to have some tools that allow us to

710 work at a higher level, defining cost functions like ?? that we defined in the  
 711 section about quantum annealing (??).

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

718 **5.4.1 PyQUBO**

719 Reading from the documentation on the PyQUBO site<sup>2</sup>, PyQUBO allows  
 720 us to create QUBOs or Ising models from flexible mathematical expressions  
 721 easily. Some of the features of PyQUBO are:

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

726 We can install PyQUBO with `pip install pyqubo` and rewrite our MVC  
 727 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'), Binary('D'),
5    ↳ 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:** Rewriting MVC with pyQUBO

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

728 Listing 5 presents a possible re-implementation of listing 4, where we also  
 729 see how PyQUBO interfaces with the Ocean SDK (line 17), and how to create  
 730 (lines 14–16) and instantiate (line 17) a parametric Hamiltonian.

731 **5.4.2 qubovert**

732 As written in the documentation<sup>3</sup>, qubovert is the one-stop package for for-  
 733 mulating, simulating, and solving problems in boolean and spin form. Using  
 734 our nomenclature, boolean and spin form are respectively QUBO and Ising  
 735 form.

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

739 **QUBO**: Quadratic Unconstrained Boolean Optimization;  
 740 **QUSO**: Quadratic Unconstrained Spin Optimization (Ising model);  
 741 **PUBO**: Polynomial Unconstrained Boolean Optimization;  
 742 **PUSO**: Polynomial Unconstrained Spin Optimization;  
 743 **PCBO**: Polynomial Constrained Boolean Optimization;  
 744 **PCSO**: Polynomial Constrained Spin Optimization.

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

```

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

**Listing 6:** Rewriting MVC with qubovert

---

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

747 Listing 6 shows a possible implementation of the MVC problem using the  
748 tools provided by qubovert. Qubovert allows us to express our problem as a  
749 PCBO; we use this formulation to express constraints in a more natural way.  
750 In our example we ensure that each edge is covered simply by enforcing that  
751 at least one of the nodes linked by the edge is present in the solution. This  
752 constraint is repeated for each edge in the graph (lines 7–13). To specify the  
753 Lagrange multiplier (equation ??) we use the keyword `lam`.

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

## 757 5.5 CONCLUSION

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

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

764    **6** | QA-PROLOG

765    **6.1 THE PROJECT**

766    **6.2 PIPELINE**

767    **6.3 UPDATE TO THE PROJECT**

768    **6.4 RELATED WORK**

769    **6.5 CONCLUSION**



770

## Part III

771

## EXPERIMENTS



<sup>772</sup> **7** | A QUANTUM ONTOLOGY

<sup>773</sup> **7.1** ONTOLOGY STRUCTURE

<sup>774</sup> **7.2** PROLOG VERSION

<sup>775</sup> **7.3** INFERENCE ON THE ONTOLOGY

<sup>776</sup> **7.4** CONCLUSION



<sup>777</sup> **8** | QAOA

<sup>778</sup> **8.1 QAOA**

<sup>779</sup> **8.2 FROM QUBO TO PAULI OPERATOR**

<sup>780</sup> **8.3 EXPERIMENTS**

<sup>781</sup> **8.4 CONCLUSION**



782 | 9 CONCLUSION