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Quantum Computing

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Information and Contacts

Personal notes and summaries collected as part of the *Quantum Computing* course offered by the degree in Computer Science of the University of Rome "La Sapienza".

Further information and notes can be found at the following link:

<https://github.com/aflaag-notes>. Anyone can feel free to report inaccuracies, improvements or requests through the Issue system provided by GitHub itself or by contacting the author privately:

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1

Introduction on Quantum Computation

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Quantum computing is a rapidly developing discipline that explores how the laws of quantum mechanics can be used to *process information*. While classical computation is based on *bits* that take values of either 0 or 1, quantum computation relies on quantum bits, or **qubits**. A qubit can exist in a “superposition” of classical states, allowing it to encode richer information than a single bit. Furthermore, qubits can exhibit particular properties that enable forms of information processing with no classical counterpart. Such properties provide the foundation for algorithms that promise to solve certain problems more efficiently than their classical analogues.

The design of quantum algorithms requires a different perspective from that of classical computation. In classical computer science, the majority of widely studied algorithms are *deterministic*, meaning that for a given input they will always produce the *same output*. Some algorithms are *randomized*, making use of probability to achieve efficiency or simplicity, yet even in those cases the computation itself is ultimately classical in nature. In fact, to achieve such *randomness* classical algorithms employ **pseudo-random number generation**, which must ultimately produce finite sequences.

Quantum computation, by contrast, *incorporates probability* at its core. The act of measuring a quantum system does not reveal a single, predetermined result, but rather yields one outcome from a distribution of possible outcomes, with probabilities governed by the system’s quantum state. This fundamental probabilistic characteristic distinguishes quantum algorithms from their classical counterparts.

In fact, in the context of quantum computing we are often interested in **probabilistic algorithms**: for such algorithms, a given input i can lead to a finite set of possible outputs o_1, \dots, o_N , each occurring with an associated probability p_1, \dots, p_N — where $\sum_{i=1}^n p_i = 1$.

introduction
on QM

1.1 The Qubit

First, we will introduce the **qubit**, the quantum equivalent of the classical bits. First, consider the following vectors: these are called **basis states**

$$|0\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and they represent the classical bits 0 and 1 respectively — the notation above is called “braket” notation and it will be explored in greater detail in the following chapter.

So what is a qubit? A qubit is the basic unit of information in quantum computing, which represents a **superposition** of states simultaneously. Mathematically speaking, the state of a qubit is a vector

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

where $\alpha, \beta \in \mathbb{C}$ such that $|\alpha|^2 + |\beta|^2 = 1$ are called **probability amplitudes**. But why are we talking about probabilities in the first place? The “true” state of a qubit **cannot be observed**, and we say that the qubit is in a *superposition* of $|0\rangle$ and $|1\rangle$ in the sense that α and β describe the probabilities of getting either states once the qubit is measured. This is because to know the value of a qubit we have to *measure it*, and the measurement operation itself will make the qubit *collapse* into either $|0\rangle$ or $|1\rangle$ with probabilities $|\alpha|^2$ and $|\beta|^2$ respectively, i.e.

$$\Pr[\text{measured qubit is } |0\rangle] = |\alpha|^2 \quad \Pr[\text{measured qubit is } |1\rangle] = |\beta|^2$$

To use a more compact notation, we will denote this property as follows:

$$\alpha|0\rangle + \beta|1\rangle \left\{ \begin{array}{ll} |0\rangle & @ |\alpha|^2 \\ |1\rangle & @ |\beta|^2 \end{array} \right.$$

where the @ notation (read as “at”) denotes the probability of the corresponding outcome. Note that if we measure a collapsed qubit we will keep observing the same state indefinitely.

In reality, to be precise qubits actually collapse into any multiple $z|0\rangle$ or $z|1\rangle$, where $z \in \mathbb{C}$ is a complex number such that $|z| = 1$, but this is not relevant from a physical point of view. In fact, for any θ physicists treat $|\psi\rangle = |0\rangle$ and $|\psi'\rangle = e^{i\theta}|0\rangle$ as the *same physical state*, because probabilities depend on squared magnitudes and thus

$$|e^{i\theta}\alpha|^2 = |\alpha|^2$$

(and the same applies for β too) even though $|\psi\rangle$ and $|\psi'\rangle$ are different vectors mathematically. Therefore, in general we can actually drop the **global phases** from the qubits entirely.

1.2 Qubit operations

What can we do with qubits other than *measure them*? The operations that can be applied on qubits are restricted to **unitary transformations**, which are linear maps that *preserve the norms* — we will discuss the precise definition of this concept in the next chapter. For instance, the identity matrix I is an example of trivial unitary transformation, but also the NOT matrix

$$\text{NOT} := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which has the effect of *swapping* the input basis state

$$\text{NOT} |0\rangle = |1\rangle \quad \text{NOT} |1\rangle = |0\rangle$$

is a unitary transformation. Note that this matrix behaves as the classical NOT gate acting on bits in classical computations, in fact will we refer to *transformations* and *gates* interchangeably.

More in general, the NOT operation belongs to a family of operations represented by the so called **Pauli matrices**.

Definition 1.1: Pauli matrices

The **Pauli matrices** are the following four 2×2 matrices:

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In particular, we observe that the second matrix σ_x is exactly the matrix of the NOT operator. For this reason, the NOT operator is also called X , and we will see the Z and Y operators (representing the other two matrices, respectively) as well in later sections.

Another very important transformation is represented by the **Hadamard gate**, which is the following matrix

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

This matrix has the effect of “mapping” classical states into superpositions:

$$H |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \left\{ \begin{array}{l} |0\rangle @ \frac{1}{2} \\ |1\rangle @ \frac{1}{2} \end{array} \right.$$

For instance, in this example given $|0\rangle$ which represents the classical bit 0, we get a qubit as output of the linear transformation. In general, the operation performed by the Hadamard gate can be represented as follows:

$$\forall a \in \{0, 1\} \quad \frac{1}{\sqrt{2}} (|0\rangle + (-1)^a |1\rangle)$$

As a side note, as we mentioned at the beginning of the chapter quantum mechanics has randomness intrinsically, and since the operation $H |0\rangle$ returns a qubit that has 50% of

probability of being either $|0\rangle$ or $|1\rangle$ once measured, this operation provides a true random number generator.

Lastly, can we *represent* qubits graphically? Well, we may be tempted to answer negatively to this question, since a qubit is described by two complex numbers $\alpha, \beta \in \mathbb{C}$, which implies that we actually need 4 dimensions to correctly represent our vector. However, through polar coordinates we can actually define a graphical representation which allows us to “picture” qubits, through the so called **Bloch sphere**. First, consider a qubit

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

for some $\alpha, \beta \in \mathbb{C}$ such that $|\alpha|^2 + |\beta|^2 = 1$, as usual. Now, recalling that any complex number $z \in \mathbb{C}$ can be actually written as follows

$$z = |z| e^{i\theta}$$

for some angle θ , we can rewrite our qubit as follows:

$$\begin{aligned} |\psi\rangle &= |\alpha| e^{i\theta_\alpha}|0\rangle + |\beta| e^{i\theta_\beta}|1\rangle \\ &= e^{i\theta_\alpha} \left(|\alpha| |0\rangle + |\beta| e^{i(\theta_\beta - \theta_\alpha)} |1\rangle \right) \\ &= |\alpha| |0\rangle + |\beta| e^{i(\theta_\beta - \theta_\alpha)} |1\rangle \quad (e^{i\theta_\alpha} \text{ is a global phase}) \\ &= |\alpha| |0\rangle + e^{i\varphi} |1\rangle \quad (\text{let } \varphi := \theta_\beta - \theta_\alpha \in [0, 2\pi)) \end{aligned}$$

and finally, since $|\alpha|^2 + |\beta|^2 = 1$ is precisely the equation of the circumference of radius 1, we usually rewrite the last equation as follows:

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\varphi} \sin\left(\frac{\theta}{2}\right)|1\rangle$$

where $\theta \in [0, \pi]$, $\varphi \in [0, 2\pi)$. This formulation of the qubit $|\psi\rangle$ allows us to represent it inside the Bloch sphere: in fact, in this formulation the qubit is normalized, which implies that it will lie on a 3 dimensional unit sphere, and it is described by the two phases θ and φ — in 2D polar coordinates there is only 1 angle, as in 3D polar coordinates there are 2 angles.

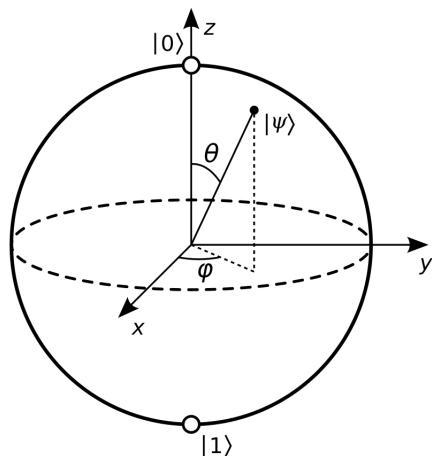


Figure 1.1: The Bloch sphere representing some qubit.

1.2.1 The tensor product

So far we have dealt with only one qubit at a time, but what if we have two qubits? First, let's look at the classical counterpart. If we take two bits $a, b \in \{0, 1\}$, we can represent 4 possible binary numbers, namely 00, 01, 10 and 11, which we can algebraically obtain by computing the usual cartesian product

$$\{0, 1\}^2 = \{0, 1\} \times \{0, 1\} = \{(0, 0), (0, 1), (1, 0), (1, 1)\}$$

Note that in the cartesian products it holds that:

- the length of the tuples of the product is linear w.r.t. the number of factors of the cartesian products — in this case, 2
- each element of a tuple is *independent* from the other elements of the tuple

How can we evaluate all the possible states that two qubits can represent, instead? To answer this question, we need to introduce a new operator, which is called **tensor product**.

Given two vectors $\begin{pmatrix} a \\ b \end{pmatrix}$ and $\begin{pmatrix} c \\ d \end{pmatrix}$, their tensor product is defined as follows

$$\begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} := \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}$$

Hence, consider two qubits

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \quad |\phi\rangle = \beta_0 |0\rangle + \beta_1 |1\rangle = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

To obtain all the possible states of $|\psi\rangle$ and $|\phi\rangle$ we just have to compute the tensor product between them, which is

$$\begin{aligned} |\psi\rangle \otimes |\phi\rangle &= \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \otimes \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \\ &= \begin{pmatrix} \alpha_0\beta_0 \\ \alpha_0\beta_1 \\ \alpha_1\beta_0 \\ \alpha_1\beta_1 \end{pmatrix} \\ &= \alpha_0\beta_0 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \alpha_0\beta_1 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \alpha_1\beta_0 \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \alpha_1\beta_1 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \end{aligned}$$

At the beginning of the chapter we defined $|0\rangle$ and $|1\rangle$ to be $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ without providing an explanation; now that we are dealing with more than 2 dimensions we can

show why such names are used. In fact, we will use the following naming convention

$$|00\rangle := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |01\rangle := \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |10\rangle := \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |11\rangle := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

and in general it holds that

$$|\text{bin}(i)\rangle = e_i$$

where $\text{bin}(i)$ represents the binary representation of i , and e_i is the i -th vector of the canonical basis. This implies that we can rewrite the previous tensor product as follows:

$$|\psi\rangle \otimes |\phi\rangle = \alpha_0\beta_0|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \alpha_1\beta_1|11\rangle = \sum_{i,j \in \{0,1\}} \alpha_i\beta_j|i j\rangle$$

where the last sum comes from the fact that

$$\forall i, j \in \mathbb{B} \quad |i\rangle \otimes |j\rangle = |i j\rangle$$

In general, we will follow this convention:

- if we write $|b\rangle$ where b is a binary string $b \in \mathbb{B}^n$ for some length n , we are referring to a vector of the canonical basis — something like $|01\rangle$, $|0\rangle$, $|110\rangle$ etc.
- if we write $|x\rangle$, $|y\rangle$, $|a\rangle$ or any other latin letter inside the label of the “braket” notation, we implicitly mean that x , y and a are treated as binary numbers and these vectors are to be intended still as elements of the canonical basis
- if we write $|\psi\rangle$, $|\phi\rangle$ or any other greek letter inside the label of the “braket” notation, we are referring to a *superposition* of basis states — something like

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

The basis of the 2D space formed by $|0\rangle$ and $|1\rangle$ is usually called **computational basis**, since we can directly map $|0\rangle$ to the classical 0, and $|1\rangle$ to the classical 1. Alternatively, it is also called **Z basis**, as opposed to the **X basis** which we will encounter in the next chapters.

Let's do an example of tensor product between two qubits defined in the Z basis: consider

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \quad |\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

When computing their tensor product we get that

$$\begin{aligned}
 |\psi\rangle \otimes |\phi\rangle &= \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \otimes \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \\
 &= \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \\
 &= \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle) \\
 &\quad \left\{ \begin{array}{ll} |0\rangle \text{ and } |0\rangle & @ \frac{1}{4} \\ |0\rangle \text{ and } |1\rangle & @ \frac{1}{4} \\ |1\rangle \text{ and } |0\rangle & @ \frac{1}{4} \\ |1\rangle \text{ and } |1\rangle & @ \frac{1}{4} \end{array} \right.
 \end{aligned}$$

where the probabilities at the end refer to the two individual qubits. To recap, in general the tensor product $|\psi\rangle \otimes |\phi\rangle$ of two qubits encodes the superposition of 4 basis states, namely $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$.

Moreover, the following property can be proved easily.

Proposition 1.1: Distributive property of \otimes

Given three qubits $|\psi\rangle$, $|\phi\rangle$ and $|\chi\rangle$, it holds that

$$(|\psi\rangle + |\phi\rangle) \otimes |\chi\rangle = |\psi\rangle \otimes |\chi\rangle + |\phi\rangle \otimes |\chi\rangle$$

1.2.2 Controlled operations

Another family of very important gates in quantum computing is the *controlled operators*, but first let's define them classically. The first controlled operation that we are going to discuss is the **Controlled NOT (CNOT)** gate, which is defined as follows:

a	b	$\text{CNOT}(a, b)$
0	0	0
0	1	1
1	0	1
1	1	0

The name comes from the fact that the first input a is called *control bit*, which if set to 1 will flip the *target bit* b . Therefore, in general we have that

$$\text{CNOT}(a, b) = a \oplus b$$

First, we observe that this function is clearly *not invertible*, since for instance if we know that the output is 0 we still need the input a to evaluate if b was 0 or 1. Hence, because we

would like this computation to be invertible — and we will see why later in our discussion — to solve this issue we usually pair the output of CNOT with a itself, so that we can actually invert the computation:

$$\text{CNOT}(a, b) = (a, a \oplus b)$$

We will start from this operator in order to construct its equivalent quantum gate.

So far we only dealt with transformations that expected only 1 qubit argument as input, but the CNOT gate would certainly need 2 inputs to perform any computation, so how do we provide two inputs to it? As we showed before, we know that

$$\forall i, j \in \{0, 1\} \quad |i\rangle \otimes |j\rangle = |ij\rangle$$

which directly implies that the vector $|ij\rangle$ encapsulates two qubits at once *without ambiguity*. Hence, we can actually leverage the tensor product to provide the input to the CNOT matrix, such that the quantum CNOT will behave as follows

$$\text{CNOT}(|a\rangle \otimes |b\rangle) = |a\rangle \otimes |a \oplus b\rangle$$

The matrix that behaves as such is the following

$$\text{CNOT} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

which expects a 4×1 input vector, and outputs a 4×1 output vector as well. Lastly, as for the CNOT operator, we can actually define controlled operators for both Y and Z, which are respectively called CY and CZ operators.

1.2.3 Quantum circuits

Now that we introduced a couple of quantum gates, we can show how computation is actually represented in quantum computing. For instance, consider the following picture:



Figure 1.2: The NOT gate.

In this example, we have 1 single input qubit, namely q , and the box labeled with an X represents the NOT gate. We observe that, by convention, all qubits in quantum circuits are assumed to be set to $|0\rangle$.

In the following example, instead, it is represented how the Hadamard gate looks like in quantum circuits.



Figure 1.3: The Hadamard gate.

Moreover, if we consider two qubits as inputs q_0 and q_1 , we can represent the CNOT operator as follows:



Figure 1.4: The CNOT gate.

We observe that q_1 then becomes the output of the CNOT operation, and q_0 remains unchanged. Lastly, the measurement operation is represented with the following picture:

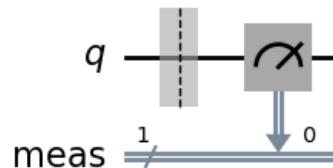


Figure 1.5: The measure operation.

In particular, in this circuit we see that:

- the vertical “double line” represents a *measured state* — which we usually call *classical wire* (even if it’s still a qubit) because it became either $|0\rangle$ or $|1\rangle$
- the number 1 next to the label `meas` indicates the number of qubits that have been measured
- the number 0 is the index of the measured qubit



Figure 1.6: An example of measurement of 2 qubits.

Lastly, another very important circuit is the following, which produces the so called **Greenberger-Horne-Zeilinger (GHZ)** state



Figure 1.7: The GHZ quantum circuit.

which is represented as follows

$$|\text{GHZ}\rangle := \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$$

All of these examples were drawn using [Qiskit](#), which is a very popular framework that is used to describe quantum computation.

1.3 Peculiarities of quantum mechanics

1.3.1 Quantum entanglement

Consider the following quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)$$

Can this state be rewritten as the tensor product of two distinct quantum states? We observe that for this to be possible we would require some complex values $\alpha_0, \alpha_1, \beta_0, \beta_1$

such that

$$\begin{cases} \alpha_0\beta_0 = \alpha_1\beta_1 = 0 \\ \alpha_0\beta_1 = \alpha_1\beta_0 = \frac{1}{\sqrt{2}} \end{cases}$$

but $\alpha_0\beta_0 = 0$ implies that at least one between α_0 and β_0 has to be 0, meaning that at least one between $\alpha_0\beta_1$ and $\alpha_1\beta_0$ has to be 0 as well. This proves that there is no such pair of quantum states which can describe $|\psi\rangle$ through the tensor product operation. In fact, we see that

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \begin{cases} |01\rangle @ \frac{1}{2} \\ |10\rangle @ \frac{1}{2} \end{cases}$$

Indeed, the choice of $|\psi\rangle$ was not a coincidence, as it is one of the so called **Bell states**.

Definition 1.2: Bell states

The following are the four **Bell states**:

$$|\Phi^+\rangle := \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

$$|\Phi^-\rangle := \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle)$$

$$|\Psi^+\rangle := \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)$$

$$|\Psi^-\rangle := \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$$

Whenever we have a state $|\psi\rangle$ that cannot be represented as the tensor product of two simpler quantum states, we say that the state is **entangled** — or that its possible outcomes are entangled. In particular, entangled states describe a very weird phenomenon first proposed as a thought experiment in a groundbreaking paper by **Einstein, Podolsky and Rosen (EPR)** [EPR35], the so called **EPR paradox**.

The thought experiment involves a pair of particles prepared in such *entangled state*. Einstein, Podolsky, and Rosen pointed out that, in this state, if the position of the first particle were measured, the result of measuring the position of the second particle *could be predicted*. If instead the momentum of the first particle were measured, then the result of measuring the momentum of the second particle could be predicted. Einstein famously called this phenomenon “spooky action at a distance”, and to the best of our knowledge the theory of quantum mechanics says that if we have two entangled states, and measure one of them — for instance, say that it collapses to $|0\rangle$ — the other state will **instantaneously** collapse to $|1\rangle$ (and viceversa). They are *perfectly anti-correlated*, even if the two states are physically light-years away from each other. For instance, in our previous example with $|\psi\rangle$ (which we now know is actually $|\Psi^+\rangle$) is that if we have two qubits q_0 and q_1 such that their *total state* is $|\psi\rangle$, whenever we measure one of them it will collapse in either $|01\rangle$ or $|10\rangle$ with 50%, and the other qubit will collapse with the

opposing outcome.

To be precise, entanglement is *not* a way to transfer information — collapsing happens instantaneously, which would violate the fact that nothing can travel faster than light, not even information. Instead, it is a way to share correlations nonlocally. In fact, it is a phenomenon that regards the *whole quantum system* considered: for instance, given three qubits q_0, q_1, q_2 , such that q_1 and q_2 are entangled, we might want to only measure $q_0 \otimes q_1$, which in turn will make q_2 collapse into some quantum state that has to be mathematically computed in order to be predicted — this will be more clear when we will describe **quantum teleportation** in [Section 1.3.2](#).

To finish off this section, we can actually generate entangled states, or **EPR pairs** for short, through quantum gates as such:



Figure 1.8: The quantum circuit for $|\Phi^+\rangle$.

In particular, we observe that the first Hadamard gate will transform $|0\rangle$ to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and through the CNOT operation we obtain

$$|\Phi^+\rangle := \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

1.3.2 Quantum teleportation

An operation that we take for granted in classical computation is the possibility to *copy* the value of a bit: if Alice has two bits $x, y \in \{0, 1\}$, and she wants to copy the value of x into y , she can do it without any issues. However, in quantum mechanics this is not so straightforward. In 1982 Wootters and Zurek [WZ82] proved the so called **No-cloning theorem**, which states that it is impossible to create an independent and identical copy of an arbitrary quantum state. However, in order to state the theorem properly we need to introduce a lot of mathematical tools which will be discussed in the following chapter. We will prove the theorem formally in [Section 5.1.1](#), but for now we will assume that cloning an arbitrary $|\psi\rangle$ is *not* possible.

Hence, if quantum states cannot be cloned, can we at least *send* them? Suppose that Alice wants to send Bob $|\psi\rangle$, described by some α and β . Clearly, the only thing that Bob has to receive are indeed the probability amplitudes of $|\psi\rangle$, so even if Alice cannot clone her quantum state, nothing prevents her to build a quantum circuit which allows Bob to receive α and β — at the cost of “destroying” her $|\psi\rangle$, i.e. measuring it. This

process is called **quantum teleportation**, and can be achieved through the following algorithm.

Algorithm 1.1: Quantum Teleportation algorithm

Given three qubits q_0 , q_1 and q_2 , the algorithm moves the state of q_0 into q_2 .

```

1: function QUANTUMTELEPORTATION( $q_0, q_1, q_2$ )
2:    $q_1 \leftarrow H(q_1)$ 
3:    $q_2 \leftarrow CX(q_1, q_2)$                                  $\triangleright$  entangle  $q_1$  and  $q_2$ 
4:    $q_1 \leftarrow CX(q_0, q_1)$ 
5:    $q_0, q_1 \leftarrow \text{measure}(q_0, q_1)$ 
6:   if  $q_1 == |1\rangle$  then
7:      $q_2 \leftarrow X(q_2)$ 
8:   end if
9:   if  $q_0 == |1\rangle$  then
10:     $q_2 \leftarrow Z(q_2)$ 
11:   end if
12:   return  $q_2$ 
13: end function
```

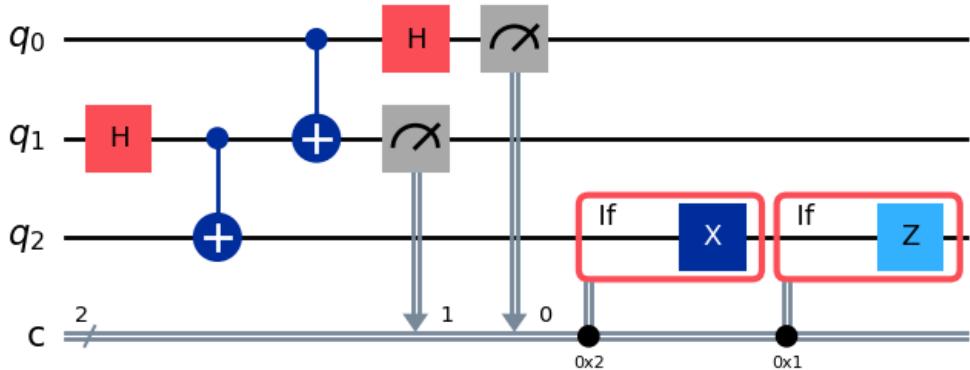


Figure 1.9: The Quantum Teleportation circuit, drawn with Qiskit.

There is quite a lot to unpack in this diagram. First, the quantum state that we want to teleport is q_0 , and it will be teleported in q_2 at the end of the quantum computation.

In the first part of the circuit, we see that q_1 and q_2 are entangled (in an initial stage of the process, not performed by Alice nor Bob) in the Bell state $|\Phi^+\rangle$ thanks to the Hadamard and the CNOT gates — as we described in previous sections. In a real-world scenario, we will assume that q_1 and q_2 are given to Alice and Bob respectively (through some **quantum channel** such as optical fibers or free-space links in order to avoid *decoherence*), and quantum mechanics will guarantee that the teleportation will work even if our two

protagonists are thousands of kilometers away from each other.

After creating and entangling q_1 and q_2 (say for instance in a lab as preparation), we have the part of circuit that concerns Alice: in fact, she must apply a CNOT to her entangled qubit q_1 , controlled by q_0 , and then apply a Hadamard transformation to q_0 . At this point, the circuit must apply a measurement to both q_0 and q_1 — and in particular, this operation will *destroy* the original state as previously anticipated.

Finally, it's Bob's turn: to obtain the original quantum state of q_0 , the only thing he needs to do is first apply a CNOT to his entangled qubit q_2 , controlled by q_1 's outcome, followed by an application of a CZ, controlled by q_0 's outcome instead — we observe that this part is indicated in the diagram through the `0x2` and `0x1` labels respectively. In fact, in the label `0xX` the number X represents the hexadecimal representation of the binary number obtained by joining the classical bits all together; for instance, in this circuit we have that `0x2` represents 10, meaning that only q_1 will be checked in the condition, and `0x1` represents 01, which means that only q_0 will be the control bit.

To show why the circuit actually works, we first need to discuss how computations with qubits and quantum gates is performed. In particular, we do not consider qubits *individually*, but instead we consider the whole **system** of qubits, i.e. $q_0 \otimes q_1 \otimes q_2$ simultaneously, and thus we will perform calculations as such. In fact, even if the drawing represents Alice's measurements of q_0 and q_1 independently, what happens in reality is that Alice is going to measure $q_0 \otimes q_1$ such that q_3 will collapse into its opposite.

Finally, we are ready to prove the correctness of the quantum teleportation circuit. Say that the qubit that Alice wants to send is

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

Then, we have that

$$\begin{aligned} & q_0 \otimes q_1 \otimes q_2 \\ &= |\psi\rangle \otimes |\Phi^+\rangle \\ &= (\alpha|0\rangle_0 + \beta|1\rangle_0) \otimes \frac{1}{\sqrt{2}}(|00\rangle_{12} + |11\rangle_{12}) \\ &= \frac{1}{\sqrt{2}}[\alpha|0\rangle_0 \otimes (|00\rangle_{12} + |11\rangle_{12}) + \beta|1\rangle_0 \otimes (|00\rangle_{12} + |11\rangle_{12})] \end{aligned}$$

where the notation $|00\rangle_{12}$ represents for example that we are considering q_1 and q_2 's parts of states, respectively. From now on, we will omit the \otimes symbol — as for the “normal” product. The next step is to apply the CNOT on q_0 and q_1 , therefore the quantum state of the system becomes the following:

$$\frac{1}{\sqrt{2}}[\alpha|0\rangle_0(|00\rangle_{12} + |11\rangle_{12}) + \beta|1\rangle_0(|10\rangle_{12} + |01\rangle_{12})]$$

Next, we have to apply the Hadamard gate on q_0 , which turns the quantum state into the

following

$$\begin{aligned}
 & \frac{1}{\sqrt{2}} \left[\alpha \frac{1}{\sqrt{2}} (|0\rangle_0 + |1\rangle_0) (|00\rangle_{12} + |11\rangle_{12}) + \beta \frac{1}{\sqrt{2}} (|0\rangle_0 - |1\rangle_0) (|10\rangle_{12} + |01\rangle_{12}) \right] \\
 & = \frac{1}{2} [\alpha (|000\rangle_{012} + |011\rangle_{012} + |100\rangle_{012} + |111\rangle_{012}) + \beta (|010\rangle_{012} + |001\rangle_{012} - |110\rangle_{012} - |101\rangle_{012})] \\
 & = \frac{1}{2} [|00\rangle_{01} (\alpha |0\rangle_2 + \beta |1\rangle_2) + |01\rangle_{01} (\beta |0\rangle_2 + \alpha |1\rangle_2) + |10\rangle_{01} (\alpha |0\rangle_2 - \beta |1\rangle_2) + |11\rangle_{01} (\alpha |1\rangle_2 - \beta |0\rangle_2)] \\
 & = \frac{1}{2} [|00\rangle_{01} |\psi\rangle_2 + |01\rangle_{01} X |\psi\rangle_2 + |10\rangle_{01} Z |\psi\rangle_2 + |11\rangle_{01} XZ |\psi\rangle_2]
 \end{aligned}$$

Finally, Alice will perform the measurement on q_0 and q_1 , and what will happen is that the *whole* quantum state of the quantum circuit will collapse as follows:

$$\left\{ \begin{array}{ll} |00\rangle_{01} \otimes |\psi\rangle_2 & @ \frac{1}{4} \\ |01\rangle_{01} \otimes X |\psi\rangle_2 & @ \frac{1}{4} \\ |10\rangle_{01} \otimes Z |\psi\rangle_2 & @ \frac{1}{4} \\ |11\rangle_{01} \otimes XZ |\psi\rangle_2 & @ \frac{1}{4} \end{array} \right.$$

In fact, from this table we can easily explain the last part of the quantum teleportation circuit, i.e. Bob's part, as shown below.

Alice's outcome	Bob's part	Bob's result
0 and 0	I	$ \psi\rangle$
0 and 1	X	$XX \psi\rangle = \psi\rangle$
1 and 0	Z	$ZZ \psi\rangle = \psi\rangle$
1 and 1	XZ	$XZXZ \psi\rangle = \psi\rangle$

Thus, in the end Bob was able to reconstruct $|\psi\rangle$ correctly, at the cost of having measured q_0 , which means that Alice lost her superposition of states forever.

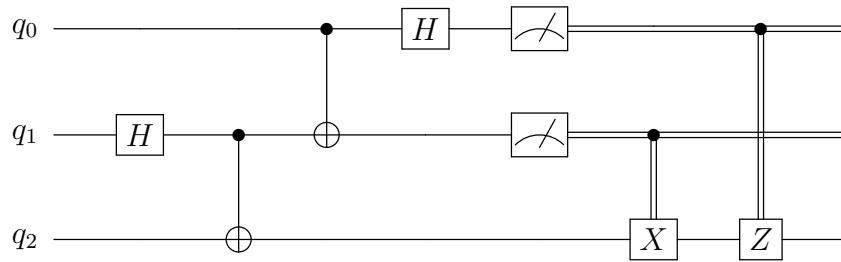


Figure 1.10: The Quantum Teleportation circuit.

As a final note, we observe that the circuit written in this form is rather unusual. Indeed, it helps to visualize the fact that Alice performs the measurement before Bob can have his qubit collapse, but in reality the measurement could have been done at the end of the circuit and it would not have made any difference at all.



Figure 1.11: The Quantum Teleportation circuit with the measurement moved at the end.

Indeed, all the quantum circuits we will present from now on will have their measurements placed at the end of the whole computation. This idea is summed up below.

Principle 1.1: Principle of deferred measurement

Measurement can always be moved from an intermediate stage of a quantum circuit to the end of the circuit. If the measurement results are used at any stage of the circuit then the classically controlled operations can be replaced by conditional quantum operations.

Algorithmically, this means that the following sequence of operations on two qubits q_0 , q_1

- 1: $b \leftarrow \text{measure}(q_0)$
- 2: **if** b **then**
- 3: $q_1 \leftarrow U(q_1)$
- 4: **end if**

which performs an application of the U gate *classically conditioned* on the result of b , can be equivalently rewritten as

- 1: $q_0, q_1 \leftarrow \text{C-}U(q_0, q_1)$
- 2: $b \leftarrow \text{measure}(q_0)$

assuming that $\text{C-}U$ is the *controlled* version of the U gate. Let's prove that this is true. Assume that the complete state of the system $|\psi\rangle$ is equal to

$$q_0 \otimes q_1 = \alpha_0 |00\rangle + \alpha_1 |01\rangle + \alpha_2 |10\rangle + \alpha_3 |11\rangle$$

Note that this is the most general case, since q_0 and q_1 might be entangled so it might not be possible to treat them separately. Thus, in the first case we have that after measuring q_0 the state becomes

$$|\psi\rangle \begin{cases} |0\rangle \otimes (\beta_{00} |0\rangle + \beta_{01} |1\rangle) & @ |\alpha_0|^2 + |\alpha_1|^2 \\ |1\rangle \otimes (\beta_{10} |0\rangle + \beta_{11} |1\rangle) & @ |\alpha_2|^2 + |\alpha_3|^2 \end{cases}$$

for some probability amplitudes β_{ij} . Then, with the application of U conditioned of the outcome of the measurement the state becomes

$$|\psi\rangle \left\{ \begin{array}{ll} |0\rangle \otimes (\beta_{00}|0\rangle + \beta_{01}|1\rangle) & @ |\alpha_0|^2 + |\alpha_1|^2 \\ |1\rangle \otimes (\beta_{10}U|0\rangle + \beta_{11}U|1\rangle) & @ |\alpha_2|^2 + |\alpha_3|^2 \end{array} \right.$$

It's easy to see that this very outcome of probabilities could have been achieved by first applying the controlled U gate to $|\psi\rangle$ at the beginning, getting

$$|\psi\rangle = \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|1\rangle \otimes U|0\rangle + \alpha_3|1\rangle \otimes U|1\rangle$$

and then measuring q_0 afterwards.

2

Mathematical foundations

Now that we have introduced some preliminary concepts in quantum mechanics and quantum computation, we can turn to the **mathematical foundations** that will allow us to develop a deeper understanding of the tools ahead. By the end of this chapter, we will be ready to state the postulates of quantum mechanics in a precise form. To prepare for that, we must first lay out several essential definitions and structures.

We will start our mathematical discussion with the definition of **scalar product** — we will assume the definitions of vector space, basis and linear independence are already known by the reader.

Definition 2.1: Scalar product

Given a scalar product vector space V , a **scalar product** $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{C} : (v, w) \mapsto \langle v, w \rangle$ is a function that satisfies the following properties:

- $\forall u, v, w \in V, \alpha, \beta \in \mathbb{C} \quad \langle u, \alpha v + \beta w \rangle = \alpha \langle u | v \rangle + \beta \langle u | w \rangle$
- $\forall u, v \in V \quad \overline{\langle u, v \rangle} = \langle v, u \rangle$ — where \bar{z} is the conjugate of $z \in \mathbb{C}$
- $\forall u \in U \quad \langle u, u \rangle \geq 0$ and $\langle u, u \rangle = 0$ if and only if $u = 0$

Scalar products are also called *inner product*, and are used to define many other tools on top of the vector space considered.

Proposition 2.1

For any scalar product vector space V , any scalar product satisfies the following property:

$$\forall u, v, w \in V, \alpha, \beta \in \mathbb{C} \quad \langle \alpha u + \beta v, w \rangle = \bar{\alpha} \langle u, w \rangle + \bar{\beta} \langle v, w \rangle$$

Proof. TODO



TODO

In particular, the scalar product that we are going to use for our purposes is defined as follows:

$$\forall u, v \in \mathbb{C}^n \quad \langle u, v \rangle = \sum_{i=1}^n \bar{u}_i v_i$$

In fact, we can prove that this is indeed a scalar product as follows:

- TODO _____ TODO
- TODO _____ TODO
- TODO _____ TODO

From now on, when we refer to a “scalar product” we will refer to this particular definition.

We are finally ready to explain the “braket” that we used from the beginning of the previous chapter. This notation was invented by the Nobel Prize in Physics [Paul Dirac](#), and it works as follows: first, observe that our scalar product can be rewritten as follows

$$\langle u, v \rangle = (\bar{u}_1 \cdots \bar{u}_n) \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$

To be precise, this product would yield a 1×1 matrix, which can be interpreted as a scalar. Through Dirac notation, we will write

$$\langle u, v \rangle = \langle u | v \rangle$$

where $\langle u |$ is called **bra**, and $|v \rangle$ is called **ket** (as in “bra-ket”). In other words, we have that $|v \rangle$ is just a regular column vector $v \in V$

$$|v \rangle = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$

defined over some scalar product vector space V , while $\langle u |$ is a *linear map* that acts as follows:

$$\langle \cdot | : V \rightarrow \overline{V} : (u_1 \cdots u_n) \mapsto (\bar{u}_1 \cdots \bar{u}_n)$$

Theorem 2.1: Cauchy-Schwarz inequality

Given a scalar product vector space V , it holds that

$$\forall u, v \in V \quad |\langle u | v \rangle| \leq \sqrt{\langle u | v \rangle \langle u | v \rangle}$$

where the equality holds if and only if u and v are linearly independent.

Moreover, our scalar product induces a **norm**, which is defined as follows.

Definition 2.2: Norm

Given a scalar product vector space V , the **norm** of a vector $v \in V$ is defined as follows

$$\|v\| = \sqrt{\langle v|v \rangle}$$

As usual, two vectors $u, v \in V$ are said to be **orthogonal** if $\langle u|v \rangle = 0$. This allows us to define orthonormal bases.

Definition 2.3: Orthonormal basis

Given a scalar product vector space V , a basis $\{e_1, \dots, e_n\}$ is said to be **orthonormal** if

$$\forall i, j \in [n] \quad \langle e_i | e_j \rangle = \delta_{ij}$$

where $\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$ is called **Kronecker delta**.

Let's see the Dirac notation in action. Consider an orthonormal basis $\{e_1, \dots, e_n\}$ for some scalar product vector space V ; by definition, we know that we can write any vector $u \in V$ as follows

$$u = \sum_{i=1}^n \alpha_i e_i$$

for some coefficients $\alpha_1, \dots, \alpha_n \in \mathbb{C}$. Now, we observe that for all $i \in [n]$

$$\begin{aligned} \langle e_i | u \rangle &= \langle e_i | \sum_{j=1}^n \alpha_j e_j \rangle \\ &= \langle e_i | \alpha_1 e_1 + \dots + \alpha_n e_n \rangle \\ &= \alpha_1 \langle e_i | e_1 \rangle + \dots + \alpha_n \langle e_i | e_n \rangle \\ &= \sum_{j=1}^n \alpha_j \langle e_i | e_j \rangle \\ &= \sum_{j=1}^n \alpha_j \delta_{ij} \\ &= \alpha_i \end{aligned}$$

Indeed, with the scalar product we can compute the projection of u onto the i -th vector of the basis. Hence, we can rewrite the first equation as follows:

$$|u\rangle = \sum_{i=1}^n \alpha_i |e_i\rangle = \sum_{i=1}^n \langle e_i | u \rangle |e_i\rangle$$

In particular, we observe that

$$|u\rangle = \sum_{i=1}^n |e_i\rangle \langle e_i | u \rangle \implies I = \sum_{i=1}^n |e_i\rangle \langle e_i|$$

which is a famous identity in quantum mechanics called **resolution of the identity**. In particular, this identity directly implies the following useful property. As a final note, by the properties of scalar products we also have that

$$\langle v|u \rangle = \left\langle v \left| \sum_{i=1}^n \langle e_i|u \rangle |e_i\rangle \right. \right\rangle = \sum_{i=1}^n \langle v|e_i \rangle \langle e_i|u \rangle$$

Proposition 2.2

Given a scalar product vector space V , it holds that

$$\forall u, v, w \in V \quad \langle u|v \rangle |w\rangle = (|w\rangle \langle u|) |v\rangle$$

Proof. TODO



2.1 Hilbert spaces

Now that we covered Dirac notation, we can describe what are **Hilbert spaces** — we will see why we care about this particular type of vector spaces later in the chapter. First, consider the following definitions.

Definition 2.4: Weak convergence

Given a scalar product vector space V , and a vector sequence $\{v_m\}_{m \in \mathbb{N}}$ defined over V , we say that the sequence **converges weakly** to a vector $v \in V$ if

$$\forall w \in V \quad \lim_{m \rightarrow +\infty} \langle v_m | w \rangle = \langle v | w \rangle$$

In other words, this type of convergence requires all projections of v_m along any fixed direction w to approach the projection of v . Differently, the next type of convergence is more strict.

Definition 2.5: Strong convergence

Given a scalar product vector space V , and a vector sequence $\{v_m\}_{m \in \mathbb{N}}$ defined over V , we say that the sequence **converges strongly** to a vector $v \in V$ if

$$\lim_{m \rightarrow +\infty} \|v - v_m\| = 0$$

In fact, this type of convergence requires the actual vectors of the sequence to get close *in norm* to v . We observe the following proposition.

Proposition 2.3

Given a scalar product vector space V , and a vector sequence $\{v_m\}_{m \in \mathbb{N}}$ defined over V , if the sequence converges strongly to some vector $v \in V$, it holds that

- the sequence also converges weakly
- the scalar products defined over V are continuous, i.e.

$$\forall u, v \in V \quad \langle u|v \rangle = \lim_{m \rightarrow +\infty} \langle u|v_m \rangle$$

Definition 2.6: Cauchy sequence

Given a scalar product vector space V , and a vector sequence $\{v_m\}_{m \in \mathbb{N}}$ defined over V , we say that the sequence is a **Cauchy sequence** if it holds that

$$\forall \varepsilon > 0 \quad \exists n_\varepsilon \in \mathbb{N} \quad \forall n, m > n_\varepsilon \quad \|v_n - v_m\| < \varepsilon$$

For example, let's consider the space \mathbb{R}^2 equipped with the Euclidean norm

$$\|v\| = \sqrt{x^2 + y^2}$$

Then, if we consider the following vector sequence

$$\left\{ \begin{pmatrix} \frac{1}{m} \\ \vdots \\ \frac{1}{m} \end{pmatrix} \right\}_{m \in \mathbb{N}}$$

we see that for any distinct m, n it holds that

$$\|v_m - v_n\| = \sqrt{\left(\frac{1}{m} - \frac{1}{n}\right)^2 + \left(\frac{1}{m} - \frac{1}{n}\right)^2} = \sqrt{2} \left| \frac{1}{m} - \frac{1}{n} \right|$$

Therefore, for any $\varepsilon > 0$ it suffices to take any $N > \frac{2\sqrt{2}}{\varepsilon}$ such that

$$\forall m, n > N \quad \|v_m - v_n\| < \varepsilon$$

We are finally ready to define Hilbert spaces.

Definition 2.7: Hilbert space

A **Hilbert space** is a *complete* scalar product vector space, i.e. it is a vector space

- equipped with a scalar product
- such that every Cauchy sequence converges strongly to an element in the space.

For example, the space \mathbb{R}^n is a Hilbert space. Indeed, since every finite vector space of size n is isomorphic to \mathbb{R}^n , we can immediately derive the following proposition.

Proposition 2.4

Finite-dimensional vector spaces are always complete.

2.1.1 Linear operators

Given a Hilbert space \mathcal{H} , we can define **operators** — which are nothing but linear maps.

Definition 2.8: Adjoint operator

Given a Hilbert space \mathcal{H} , and an operator A , the **adjoint** operator of A , denoted with A^\dagger , is a linear map that satisfies the following property

$$\forall u, v \in \mathcal{H} \quad \langle u | A^\dagger v \rangle = \langle Au | v \rangle$$

We say that an operator A is **self-adjoint**, or *Hermitian*, if and only if $A = A^\dagger$.

For instance, the following matrix $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$ is a linear operator whose adjoint is $S^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$. In fact, we have that

$$\langle u | S^\dagger v \rangle = (\overline{u_1} \ \ \overline{u_2}) \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = (\overline{u_1} \ \ \overline{u_2}) \begin{pmatrix} v_1 \\ -iv_2 \end{pmatrix} = \overline{u_1}v_1 - i\overline{u_2}v_2$$

and since

$$Su = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} u_1 \\ iu_2 \end{pmatrix} \implies \langle Su | v \rangle = (\overline{u_1} \ \ \overline{iu_2}) \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \overline{u_1}v_1 - i\overline{u_2}v_2$$

but because $\overline{iu_2} = \bar{i} \cdot \overline{u_2} = -i\overline{u_2}$ this implies that

$$\langle Su | v \rangle = (\overline{u_1} \ \ -i\overline{u_2}) \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \overline{u_1}v_2 - i\overline{u_2}v_2$$

Proposition 2.5

For any adjoint operators A, B defined over some Hilbert space \mathcal{H} , it holds that

1. $(AB)^\dagger = B^\dagger A^\dagger$
2. for any scalar z it holds that $(zA)^\dagger = \bar{z}A^\dagger$
3. $(A^\dagger)^\dagger = A$
4. $(A + B)^\dagger = A^\dagger + B^\dagger$

How do we evaluate the adjoint of a given operator?

Proposition 2.6

Given an operator A defined over a scalar product vector space, it holds that

$$A_{ij}^\dagger = \overline{A_{ji}}$$

This property is incredibly useful, because it implies that the adjoint operator of A is its transposed conjugate matrix. Most notably, due to the way we defined our scalar product, it holds that for any column vector $|x\rangle$ we have that

$$\langle x| = |x\rangle^\dagger$$

which gives an intuition of the reason why we defined our scalar product as such.

Proposition 2.7

If an operator A is self-adjoint, it holds that

$$\langle u|Av\rangle = \langle Au|v\rangle = \overline{\langle v|Au\rangle}$$

Proof. TODO



At the beginning of the previous chapter we said that all quantum gates are *unitary transformations*, but we did now provide a definition of unitary. Now we are ready to introduce it, and start to grasp why we are discussing Hilbert spaces.

Definition 2.9: Unitary operators

Given a Hilbert space \mathcal{H} , and an operator U , we say that U is **unitary** if it holds that

$$UU^\dagger = U^\dagger U = I$$

In other words, U is unitary if and only if its adjoint operator is also its inverse. An interesting characterization of unitary transformations is the following property.

Proposition 2.8: Unitary operators (alt. def.)

An operator U defined over a Hilbert space \mathcal{H} is unitary if and only if

- U is surjective
- $\forall x, y \in \mathcal{H} \quad \langle Ux|Uy\rangle = \langle x|y\rangle$ or equivalently, if it holds that

$$\forall x \in \mathcal{H} \quad \|Ux\| = \|x\|$$

Proof. TODO



TODO

In particular, we observe that the second property of this proposition is very interesting: the *preservation of scalar product*, i.e. the property for which

$$\forall x, y \in \mathcal{H} \quad \langle Ux | Uy \rangle = \langle x | y \rangle$$

means that the operator U does not change the geometric relationships between vectors — i.e. their lengths and angles remain the same.

Proposition 2.9

If A and B are two unitary operators, then AB is a unitary operator.

Proof. Since A and B are unitary it holds that

$$A^\dagger A = AA^\dagger = B^\dagger B = BB^\dagger = I$$

Now, by [Proposition 2.5](#) we have that

$$(AB)^\dagger = B^\dagger A^\dagger$$

from which we conclude that

$$(AB)^\dagger (AB) = B^\dagger A^\dagger AB = B^\dagger IB = B^\dagger B = I$$



Definition 2.10: Normal operators

Given a Hilbert space \mathcal{H} , and an operator A , we say that A is **normal** if it satisfies the following property

$$A^\dagger A = AA^\dagger$$

Clearly, from their definition we immediately see that both self-adjoint and unitary operators are both normal.

Lastly, say that we know that how an operator U acts on some input $|x\rangle$, and we want to derive U . How can we do this?

Proposition 2.10

For any operator U in a Hilbert space \mathcal{H} , if \mathcal{B} is a base of \mathcal{H} it holds that

$$U = \sum_{b \in \mathcal{B}} U |b\rangle \langle b|$$

Proof. The formula derives directly from the resolution of the identity, and the linearity of operators of Hilbert spaces

$$\begin{aligned} U &= U \cdot I \\ &= U \cdot \sum_{b \in \mathcal{B}} |b\rangle \langle b| \\ &= \sum_{b \in \mathcal{B}} U |b\rangle \langle b| \end{aligned}$$

□

Therefore, if we know how U acts component-wise, we can reconstruct the operator acting on the whole space as such.

2.2 Spectral theory

Since unitary operators are linear maps, we are interested in their eigenvectors and eigenvalues — which are defined as usual. First, let us recall some preliminary definitions.

Definition 2.11: Non-degenerate eigenvalue

Given a matrix A , and an eigenvalue λ of A , we say that λ is **non-degenerate** if the associated eigenspace has dimension 1 (or equivalently, if it has only 1 associated eigenvector).

Definition 2.12: d -fold degenerate eigenvalue

Given a matrix A , and an eigenvalue λ of A , we say that λ is d -fold degenerate if there are d linearly independent eigenvectors u_1, \dots, u_d associated to λ .

In Dirac notation, if λ is non-degenerate, we refer to the only eigenvector associated to λ as $|\lambda\rangle$, indeed it holds that

$$A |\lambda\rangle = \lambda |\lambda\rangle$$

Proposition 2.11

Given a matrix A defined over a Hilbert space \mathcal{H} , and an eigenvalue λ associated to A , it holds that

$$\langle \lambda | A^\dagger = \bar{\lambda} \langle \lambda |$$

Proof. TODO

□

TODO

The following theorem provides a characterization of the eigenvalues and eigenvectors of self-adjoint and unitary operators, which have surprisingly nice properties.

Theorem 2.2: Spectral theorem

The following propositions hold:

- The eigenvalues of a self-adjoint operator are real values.
- The eigenvalues of a unitary operator are complex values of modulus 1.
- Eigenvectors of self-adjoint and unitary operators associated to different eigenvalues are orthogonal to each other.

Moreover, for finite-dimensional Hilbert spaces the following holds.

Theorem 2.3: Spectral theorem for fin. Hilbert spaces

Given a finite-dimensional Hilbert space \mathcal{H} , and a normal operator A defined over \mathcal{H} , the set of all eigenvectors of A is an orthonormal basis for \mathcal{H} .

We can rewrite this theorem as follows: if we denote with u_{ij} the j -th eigenvector associated to the i -th eigenvalue of A , it holds that

$$\forall v \in \mathcal{H} \quad v = \sum_{i=1}^m \sum_{j=1}^{d_i} \alpha_{ij} u_{ij}$$

where d_i is the geometric multiplicity of the i -th eigenvalue of A . Indeed, we observe that $\dim \mathcal{H} = \sum_{i=1}^m d_i$. Lastly, through the Dirac notation we can rewrite the formula as follows

$$\forall v \in \mathcal{H} \quad |v\rangle = \sum_{i=1}^m \sum_{j=1}^{d_i} \langle \lambda_{ij} | v \rangle |\lambda_{ij}\rangle$$

2.3 Projectors

Next, we are going to discuss **projectors**, which are another very crucial pieces of quantum computation. We saw how scalar products are able to perform projection over desired direction, in fact we will use the Dirac notation to define precise operators for our purposes. But as always, first some preliminary definitions.

Definition 2.13: Orthogonal space

Given a scalar product vector space U , and two linear subspaces $V, W \subset U$, we say that V is orthogonal to W if

$$\forall v \in V, w \in W \quad \langle v | w \rangle = 0$$

Given a scalar product vector space U , and a linear subspace $V \subset U$, the **orthogonal**

complement of V is defined as follows:

$$V^\perp := \{u \in U \mid \forall v \in V \quad \langle u | v \rangle = 0\}$$

In particular, we observe that if U is finite-dimensional it holds that $V = U - V^\perp$ and that $(V^\perp)^\perp = V$.

Definition 2.14: Topologically closed subspace

Given a Hilbert space \mathcal{H} , and a linear subspace $V \subset \mathcal{H}$, we say that V is **topologically closed** if any sequence of vectors defined over V converges in V .

Interestingly enough, given a topologically closed subspace $V \subset \mathcal{H}$ of some Hilbert space, we can write any vector $u \in V$ as the sum of two orthogonal vectors of V and V^\perp , as follows. Let $\{f_1, \dots, f_n\}$ be an orthonormal basis of V , and define the following vectors

$$\forall u \in U \quad u_V := \sum_{i=1}^n \langle f_i | u \rangle f_i$$

Then, if we call

$$u_{V^\perp} := u - u_V$$

, we see that TODO which indeed proves that u_V and u_{V^\perp} are orthogonal to each other.

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With this observation, we can finally define the projector operators.

Definition 2.15: Projector

Given a Hilbert space \mathcal{H} , and a closed subspace $V \subset \mathcal{H}$, the **projector** operator that projects any given vector $v \in \mathcal{H}$ onto V is defined as follows:

$$P_V : \mathcal{H} \rightarrow V : u \mapsto u_V = \sum_{i=1}^n \langle f_i | u \rangle f_i$$

where $\{f_1, \dots, f_n\}$ is an orthonormal basis of V .

In other words, the projector we have that

$$P_V := \sum_{i=1}^n |f_i\rangle \langle f_i|$$

Clearly, by definition of u_{V^\perp} it holds that

$$P_{V^\perp} : \mathcal{H} \rightarrow V^\perp : u \mapsto u_{V^\perp} := u - u_V$$

Moreover, since P_V performs a projection, we have that

$$\forall u \in \mathcal{H} \quad u \in V \iff P_V u = u$$

and that

$$\forall u \in \mathcal{H} \quad u \in V^\perp \iff P_V u = 0$$

Additionally, for any projector P_V it holds that $P_V^2 = P_V$, by idempotency, and $P_V^\dagger = P_V$.

Proposition 2.12

Any projector operator only has 0 and 1 as possible eigenvalues.

Proof. Consider a projector operator P_V ; by definition v is an eigenvalue of P_V associated to the eigenvalue λ if it holds that

$$P_V v = \lambda v$$

Hence, we observe that

$$P_V^2 v = P_V(P_V v) = P_V(\lambda v) = \lambda P_V v = \lambda(\lambda v) = \lambda^2 v$$

and by idempotency of P_V it holds that

$$\lambda^2 v = P_V^2 v = P_V v = \lambda v$$

which implies that

$$\lambda^2 v - \lambda v = 0 \iff (\lambda^2 - \lambda)v = 0$$

Finally, since v is an eigenvector it holds that $v \neq 0$, therefore it must be that the last equation is true only if

$$\lambda^2 - \lambda = 0 \iff \lambda = 0 \vee \lambda = 1$$

□

Given a Hilbert space \mathcal{H} , and two topologically closed subspaces $V, W \subset \mathcal{H}$, we say that P_V and P_W are **orthogonal** if it holds that $V \perp W$. Now, fix a vector $u \in \mathcal{H}$; by definition $P_V u$ is a vector that lies inside V , therefore it holds that

$$P_W(P_V u) = 0$$

since $V \perp W$, and by the same reasoning applied on W first we conclude that

$$P_W P_V = P_V P_W = \mathbf{0}$$

where **0** is the **zero operator** — indeed, it is a zero matrix.

As a final note, if A is a linear operator, and λ is an eigenvalue of A , we denote with P_λ the projector that projects vectors onto the eigenspace associated to λ .

Proposition 2.13

If P and Q are two orthogonal projectors, then $P + Q$ is still a projector.

Proof. TODO

□

TODO

The following is the last property of projectors that we will present, and it will be very useful when we will introduce the postulates of quantum mechanics in the next section.

Theorem 2.4: Spectral decomposition

Given a Hilbert space \mathcal{H} , and a normal operator A defined on \mathcal{H} whose eigenvalues are $\lambda_1, \dots, \lambda_n$, the matrix A can be rewritten as follows:

$$A = \sum_{i=1}^n \lambda_i P_{\lambda_i}$$

2.4 Tensor product

Finally, the last ingredient that we need to discuss is the **tensor product**

TODO

TODO

2.5 Rules of quantum mechanics

Now that we defined Hilbert spaces and their operators in great detail, we can finally present we needed this mathematical foundations in order to progress: quantum mechanics is developed over Hilbert spaces with *countable* bases, and quantum computing works with finite-dimensional Hilbert spaces. In particular, these are the four fundamental **postulates of quantum mechanics**.

Postulate 2.1: State postulate

The state of a quantum system is completely described by a vector $|\psi\rangle$ in a Hilbert space \mathcal{H} .

As we saw at the beginning of the previous chapter, $|\psi\rangle$ is always considered to be normalized. We observe that different physical systems of different types live in different Hilbert spaces.

Postulate 2.2: Measurement postulate

Every measurable (i.e. *observable*) quantity corresponds to a self-adjoint operator on \mathcal{H} . In particular, given an observable A , and a state $v \in \mathcal{H}$, it holds that:

- the only possible results of measuring A are one of its eigenvalues
- the probability of measuring eigenvalue λ in state v is given by

$$\Pr[A = \lambda | v] = \langle v | P_\lambda v \rangle$$

where P_λ is the linear map that projects v onto the λ -eigenspace.

We can actually explain why we choose that particular scalar product to be the probability. Since by convention any quantum state is normalize, i.e. $\|v\| = 1$, it holds that

$$\begin{aligned} 1 &= \|v\|^2 \\ &= \langle v | v \rangle \\ &= \left\langle \sum_{i=1}^m P_{\lambda_i} v \middle| \sum_{j=1}^m P_{\lambda_j} v \right\rangle \\ &= \sum_{i=1}^m \sum_{j=1}^m \langle P_{\lambda_i} v | P_{\lambda_j} v \rangle \end{aligned}$$

Now, since each P_{λ_i} is a projector, we know that when $i \neq j$ it holds that $P_{\lambda_i} P_{\lambda_j} = \mathbf{0}$, therefore by self-adjointness of projectors we have that

- if $i \neq j$ then

$$\langle P_{\lambda_i} v | P_{\lambda_j} v \rangle = \langle v | P_{\lambda_i} P_{\lambda_j} v \rangle = \langle v | \mathbf{0} v \rangle = 0$$

- if $i = j$ then

$$\langle P_{\lambda_i} v | P_{\lambda_j} v \rangle = \langle P_{\lambda_i} v | P_{\lambda_i} v \rangle = \|P_{\lambda_i} v\|^2$$

Therefore, by adding only the non-zero terms we get that

$$\sum_{i=1}^m \|P_{\lambda_i} v\|^2 = 1$$

Hence, we define

$$\Pr[A = \lambda_i | v] := \|P_{\lambda_i} v\|^2$$

such that

$$\Pr[A | v] = \sum_{i=1}^m \Pr[A = \lambda_i | v] = \sum_{i=1}^m \|P_{\lambda_i} v\|^2 = \|v\|^2 = 1$$

which also means that our probabilities will add up to 1 automatically. Finally, we can

rewrite this probability as follows (we will drop the index of the eigenvalue):

$$\begin{aligned}\Pr[A = \lambda | v] &= \langle P_\lambda v | P_\lambda v \rangle \\ &= \langle v | P_\lambda^\dagger P_\lambda v \rangle \\ &= \langle v | P_\lambda^2 v \rangle \quad (\text{by self-adjointness}) \\ &= \langle v | P_\lambda P_\lambda v \rangle \\ &= \langle v | P_\lambda v \rangle\end{aligned}$$

This formulation was refined in 1926 by Max Born [Hal13], when he derived the following property.

Theorem 2.5: Born rule

The probability that a qubit $|\psi\rangle$ written in a basis $\{\lambda_i\}_{i=1}^n$ collapses to a particular $|\lambda\rangle \in \{\lambda_i\}_{i=1}^n$ when measured is

$$\Pr[\text{measure}(|\psi\rangle = |\lambda\rangle)] = |\langle\psi|\lambda\rangle|^2$$

Proof. By the [Theorem 2.3](#) it holds that the set of all the eigenvectors $|\lambda\rangle$ of any operator always form an orthonormal basis of the complete Hilbert space. Hence, the idea is to implicitly construct a self-adjoint operator A whose eigenvalues are precisely the possible values in which $|\psi\rangle$ might collapse into. In other words, we want to construct a self-adjoint operator whose [Spectral decomposition](#) is exactly defined by $\{\lambda_1, \dots, \lambda_n\}$. Hence, if $|\psi\rangle$ is defined as

$$|\psi\rangle = \sum_{i=1}^n \alpha_i |\lambda_i\rangle$$

we define the operator

$$A_\psi = \sum_{i=1}^n \lambda_i P_{\lambda_i} = \sum_{i=1}^n \lambda_i |\lambda_i\rangle \langle \lambda_i|$$

Thus, the probability that by $|\psi\rangle$ it collapses to some $|\lambda\rangle \in \{\lambda_1, \dots, \lambda_n\}$ can be rewritten as follows:

$$\begin{aligned}\Pr[\text{measure}(|\psi\rangle = |\lambda\rangle)] &= \Pr[A_\psi = \lambda | |\psi\rangle] \\ &= \langle \psi | P_\lambda \psi \rangle \quad (\text{by Postulate 2.2}) \\ &= \langle \psi | (|\lambda\rangle \langle \lambda|) \psi \rangle \\ &= \langle \psi | |\lambda\rangle \langle \lambda| \psi \rangle \\ &= (\langle \psi | \lambda \rangle)(\langle \lambda | \psi \rangle) \\ &= |\langle \psi | \lambda \rangle|^2\end{aligned}$$

□

For instance, if we have a superposition

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

and we want to know what is the probability that $|\psi\rangle$ collapses to $|0\rangle$ after a measurement, we simply have that

$$\begin{aligned}\Pr[\text{measure}(|\psi\rangle = |0\rangle)] &= \Pr[A_\psi = 0 | |\psi\rangle] \\ &= |\langle\psi|0\rangle|^2\end{aligned}$$

where the A_ψ matrix is precisely:

$$A_\psi = 0 \cdot P_0 + 1 \cdot P_1 = 0 \cdot |0\rangle\langle 0| + 1 \cdot |1\rangle\langle 1|$$

This formulation of the probability of measurements will be used extensively for our purposes, and allows us to avoid the description of the matrix A_ψ completely.

Before presenting to the next postulate, another very important operator that is frequently utilized in quantum mechanics is the **expected value** of a matrix. Given an observable A , we define the expected value of A as the average eigenvector we may obtain after a measurement

$$\mathbb{E}[A|v] = \sum_{i=1}^m \lambda_i \Pr[A = \lambda_i | v]$$

We usually denote the expected value of the operator A as $\langle A \rangle$. Moreover, we have the following property.

Proposition 2.14: Expected value of an operator

Given an Hermitian operator A , if the system is in state $|\psi\rangle$ it holds that

$$\langle A \rangle = \langle \psi | A \psi \rangle$$

Proof. By Postulate 2.2, it follows that

$$\begin{aligned}\langle A \rangle &= \mathbb{E}[A | |\psi\rangle] \\ &= \sum_{i=1}^m \lambda_i \Pr[A = \lambda_i | |\psi\rangle] \\ &= \sum_{i=1}^m \lambda_i \langle \psi | P_{\lambda_i} \psi \rangle \\ &= \sum_{i=1}^m \lambda_i \langle \psi | |\lambda_i\rangle \langle \lambda_i | \psi \rangle \\ &= \left(\sum_{i=1}^m \lambda_i \langle \psi | |\lambda_i\rangle \langle \lambda_i | \right) \psi \\ &= \left(\langle \psi | \sum_{i=1}^m \lambda_i |\lambda_i\rangle \langle \lambda_i | \right) \psi \\ &= \langle \psi | A | \psi \rangle \\ &= \langle \psi | A \psi \rangle\end{aligned}$$

□

Postulate 2.3: Time evolution postulate

A closed system evolves through time according to the **time-dependent Schrödinger equation (TDSE)**:

$$i\hbar \frac{d}{dt}v(t) = Hv(t)$$

We observe that the Schrödinger equation is a first-order linear differential equation, and it is composed by the following elements:

- $v(t)$ which is the state vector at time t (a vector in a Hilbert space)
- H which is the system *Hamiltonian*, a self-adjoint operator that describes the total energy of the system

The solution of the Schrödinger equation is

$$v(t_1) = U(t_2, t_1)v(t_1)$$

where $U(t_2, t_1)$ is called **time-evaluation operator**, and it is defined as follows:

$$U(t_2, t_1) = e^{-\frac{i}{\hbar}H(t_2-t_1)}$$

(assuming H does not depend on time). We recall that H is a matrix, so we are raising e to the power of a matrix, an operation that is defined by the power series of the exponential as follows:

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

What is interesting about this operator is that U is **unitary**, and in order to show it is suffices to prove that $U^\dagger = U^{-1}$. But how do we compute the adjoint of U ? We observe that by the properties of the adjoint operation it holds that

$$(e^A)^\dagger = \left(\sum_{n=0}^{\infty} \frac{A^n}{n!} \right)^\dagger = \sum_{n=0}^{\infty} \frac{(A^n)^\dagger}{n!} = \sum_{n=0}^{\infty} \frac{(A^\dagger)^n}{n!} = e^{A^\dagger}$$

which means that the adjoint of an exponential is the exponential of the adjoint. This suffices to prove that

$$U^\dagger = \left(e^{-\frac{i}{\hbar}H(t_2-t_1)} \right)^\dagger = e^{\left(-\frac{i}{\hbar}H(t_2-t_1) \right)^\dagger} = e^{\frac{i}{\hbar}H(t_2-t_1)} = \left(e^{-\frac{i}{\hbar}H(t_2-t_1)} \right)^{-1} = U^{-1}$$

This is a crucial characteristic for quantum mechanics: since U is unitary, we know that it preserves the scalar product by [Proposition 2.8](#), therefore it also preserves **probabilities and norms**. This is why we say that evolution in quantum systems — or *quantum evolution*, for short — is unitary.

Postulate 2.4: Composite systems postulate

If system A is defined over \mathcal{H}_A , and system B is defined over \mathcal{H}_B , the total system lives in

$$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$$

In other words, the last postulate states that the Hilbert space of a composite system is the tensor product of the Hilbert spaces of its subsystems.

3

Quantum algorithms

Now that we presented all the mathematical tools we need to perform quantum computations, we are ready to explore some of the most famous and most important quantum algorithm that have been developed in recent years. But before introducing any algorithm, let's discuss *why* we are interested in quantum computing at all.

Consider some computable function $f(x)$ and some classical algorithm that is able to compute it for any valid input x . If we have an input x_1 , and we want to compute its output we need to run the algorithm in order to compute $f(x_1)$. Analogously, if we have another input x_2 we need to run the algorithm again in order to compute $f(x_2)$. In general, if we want to know the outputs $f(x_1), \dots, f(x_N)$ of N inputs x_1, \dots, x_N , with classical computing we must the algorithm N distinct times, because there is no way to compute more than one output at a time. With quantum computations, however, we will see that not only this is possible, but we can actually compute *all* the possible outputs related to all the possible inputs **simultaneously**. To the best of our knowledge, through the laws of quantum mechanics we *really* can compute all the possible outputs $f(x)$ for each $x \in \mathbb{B}^n$ — for a fixed input length n .

How does this work in practice? Recall that we *seemingly arbitrarily* decided to denote the vectors of the canonical basis with binary strings, such as $|000\rangle$, $|001\rangle$, $|010\rangle$ and so on (we chose $n = 3$ for this example). This is no coincidence: since these vectors form a basis, we can write any quantum state $|\psi\rangle$ as a linear combination of them, and by doing so we obtain something like

$$|\psi\rangle = \sum_{x \in \mathbb{B}^3} \alpha_x |x\rangle$$

Say that we want to compute $f(x)$ for all $x \in \mathbb{B}^3$. Assuming that the function $f(x)$ can be defined with a unitary operator U (which means that U is 1 single quantum gate), by linearity of quantum operators when we apply U to $|\psi\rangle$ we get that

$$U |\psi\rangle = \sum_{x \in \mathbb{B}^3} \alpha_x U |x\rangle$$

Notice what happened here! By only applying U to $|\psi\rangle$ we actually applied U on *all the vectors of the basis simultaneously*. This explains the choice of the labeling of the vectors of the canonical basis.

So, what's the catch? Well, we also recall that superpositions of states must be measured at some point, and this is the problem: when we measure the result of $U|\psi\rangle$ we will inevitably only get 1 single value, namely $U|x\rangle$ for some $x \in \mathbb{B}^n$, with probability $|\alpha_x|^2$. This makes finding *useful* quantum algorithm extremely difficult, because even if we are performing all the computations at once we can only see the result of 1 possible output, at random. Hence, not only quantum algorithms are hard to discover because of this inherent limitation of quantum mechanics, but they must also be more efficient than any classical alternative we currently know, otherwise there is really no point in using this very complicated computing framework (both in terms of hardware and software). The algorithms that we will see in this chapter — and also in the next one — are some of the most important quantum procedures that we know, and sparked a lot of interest in this area of research in recent years.

But before starting our discussion about quantum algorithm, we need to present another peculiarity of quantum computation. When we introduced quantum operators we underlined the fact that each quantum gate has to be a *unitary* operator, and we now have the mathematical foundation to know that if a matrix is unitary, it is clearly also invertible — indeed, its adjoint is its inverse. This directly implies a very important property of quantum computation: except for the measurement operation, every quantum computation operation is **reversible**.

Truth be precise, classical computation *admits* reversible computation. In fact, we observe that we do have examples of reversible classical computation that does not lose efficiency — in terms of time. In 1963 Lecerf and Euratom [LE64] proposed a reversible Turing machine, and in 1973 a landmark result by Bennett [Ben73] proved that any standard Turing machine can be actually simulated by a reversible one — his construction involves augmenting the Turing machine with an auxiliary *history tape*, which can potentially lead to a large space overhead.

Consider the following bitwise operator T , that given three bits it works as follows:

$$T : \{0, 1\}^3 \rightarrow \{0, 1\}^3 : (a, b, c) \mapsto (a, b, c \oplus (a \wedge b))$$

The corresponding classical gate of this bitwise operator is called **Toffoli gate**, and it has very special characteristics. First, observe how it computes: while a and b remains unchanged, c is basically flipped if and only if both a and b are set to 1. In other words, both a and b act as “control bits” over the “target bit” c , indeed the Toffoli gate is sometimes called **Controlled Controlled NOT (CCNOT)**. As we did for the CNOT, this operator is clearly invertible since we are passing the bits a and b to the output too — also, the truth table of the Toffoli gate easily shows that it is indeed invertible. Moreover, we observe that by associativity of the XOR it holds that

$$(c \oplus (a \wedge b)) \oplus (a \wedge b) = c \oplus (a \wedge b) \oplus (a \wedge b) = c$$

which directly implies that

$$T^2 = I \implies T = T^{-1}$$

However, above all the most important property of the Toffoli gate is that it is **universal**. In fact, even though gates like NAND and NOR are universal too, they are *irreversible*. This implies that with the T operator we can build any reversible Boolean function, and since any ordinary Boolean function can be embedded into a reversible one — by adding extra bits to make it invertible — any classical computation can be simulated using Toffoli gates only.

3.1 Deutsch's algorithm

Even though quantum computation provides reversibility “for free”, we saw that classical computation can still achieve invertibility of computation. However, the next characteristic that we are going to describe has no classical analogue.

First, let's start with a problem seemingly unrelated to our discussion. Given a Boolean function $f : \{0, 1\}^n \rightarrow \{0, 1\}$, we would like to embed f inside a quantum computation. However, when $n \geq 3$ we are guaranteed that $f(x)$ is not reversible — it cannot be injective. This is a problem, since in quantum computing all gates must be reversible — given that quantum evolution is unitary. Thus, how do we turn f into a reversible computation?

We define a map U_f defined as follows:

$$U_f : \{0, 1\}^{n+1} \rightarrow \{0, 1\}^{n+1} : (x, y) \mapsto (x, y \oplus f(x))$$

First, we observe that

$$(y \oplus f(x)) \oplus f(x) = y \oplus (f(x) \oplus f(x)) = y$$

which trivially proves that U_f is reversible. Moreover, we can actually prove that when applied to qubits the corresponding quantum operator

$$U_f : \mathcal{H} \rightarrow \mathcal{H} : |x\rangle |y\rangle \mapsto |x\rangle |y \oplus f(x)\rangle$$

is indeed unitary — we observe that we are omitting the tensor product symbol in the function definition, as usual in the literature.

Proposition 3.1

Given a Boolean function $f : \{0, 1\}^n \rightarrow \{0, 1\}$, the operator U_f is unitary.

Proof. TODO

□ TODO

This proves that the construction of U_f is precisely the gate that allows us to embed f into any quantum computation. Moreover, we observe that

- $|y\rangle = |0\rangle \implies U_f |x\rangle |0\rangle = |x\rangle |f(x)\rangle$
- $|y\rangle = |1\rangle \implies U_f |x\rangle |1\rangle = |x\rangle |\neg f(x)\rangle$

However, until now we only considered already collapsed qubits, but what if we consider a quantum input that is in a superposition? For instance, let

$$|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

and assume that $|y\rangle = |0\rangle$ for simplicity; this implies that

$$\begin{aligned} U_f |x\rangle |y\rangle &= U_f \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle \\ &= U_f \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \\ &= \frac{1}{\sqrt{2}}(U_f |00\rangle + U_f |10\rangle) \quad (\text{by linearity of } U_f) \\ &= \frac{1}{\sqrt{2}}(|0\rangle |f(0)\rangle + |1\rangle |f(1)\rangle) \end{aligned}$$

But notice what just happened: both $f(0)$ and $f(1)$ have been computed **simultaneously**, in one gate application. This has no classical equivalent, we would have to evaluate $f(0)$ and $f(1)$ *separately*. This phenomenon is called **quantum parallelism**, and it can be achieved only because:

- qubits are in superpositions
- quantum gates are linear

However, we observe that the result of our calculations is *still a superposition*. In fact, if we measure the output of $U_f |x\rangle |y\rangle$ we would still get either $|0\rangle |f(0)\rangle$ or $|1\rangle |f(1)\rangle$, both with 50% probability. This is a problem: the fact that we can compute $f(0)$ and $f(1)$ at the same time seems promising, but can we retrieve their actual values?

Unfortunately, this is not possible. Indeed, quantum parallelism cannot help us with *local* properties — i.e. when we need all individual outputs — it can only help when we need **global** properties. This limit derives from the fact that measurements prevent “seeing” both outcomes, in fact if we were able to compute $f(0)$ and $f(1)$ simultaneously from this superposition we would be violating the laws of quantum mechanics themselves.

Then, how do we extract useful *global* information from the superposition output? In 1985 Deutsch [Deu85] defined a quantum algorithm which is able to compute $f(0) \oplus f(1)$, which clearly tells us if $f(0)$ equals $f(1)$ or not.

Algorithm 3.1: Deutsch algorithm

Given a Boolean function f and 2 qubits, the algorithm returns $|0\rangle$ if f if $f(0) = f(1)$, $|1\rangle$ otherwise.

```

1: function DEUTSCH( $f$ ,  $q_0$ ,  $q_1$ )
2:    $q_1 \leftarrow X(q_1)$ 
3:    $q_0, q_1 \leftarrow (H \otimes H)(q_0, q_1)$ 
4:    $q_0, q_1 \leftarrow U_f(q_0, q_1)$ 
5:    $q_0 \leftarrow H(q_0)$ 
6:   return measure( $q_0$ )
7: end function

```

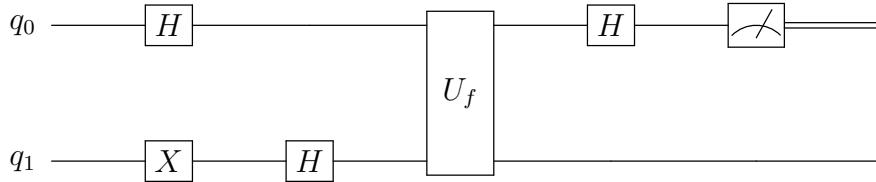


Figure 3.1: The quantum circuit for Deutsch's algorithm. The box labeled with U_f represents a “black-box” for whatever computation U_f represents (which directly depends on the choice of f).

Proving that this quantum circuit is correct, however, will be a little more involved than what we did for the quantum teleportation. First, we need a lemma that will simplify our calculations.

Lemma 3.1

For any Boolean function f defined on n bits, and $a \in \{0, 1\}^n$, it holds that

$$U_f |a\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = (-1)^{f(a)} |a\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Proof. First, by algebraic manipulation we see that

$$\begin{aligned} U_f |a\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) &= U_f \frac{1}{\sqrt{2}}(|a0\rangle - |a1\rangle) \\ &= \frac{1}{\sqrt{2}}(U_f |a0\rangle - |a1\rangle) \\ &= \frac{1}{\sqrt{2}}(|a f(a)\rangle - |a \neg f(a)\rangle) \end{aligned}$$

and now, we observe that

- if $f(a) = 0$, then

$$\frac{1}{\sqrt{2}}(|a0\rangle - |a1\rangle) = (-1)^0 |a\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

- if $f(a) = 1$, then

$$\frac{1}{\sqrt{2}}(|a1\rangle - |a0\rangle) = (-1)^1 |a\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

□

We are now ready to prove the correctness of Deutsch's algorithm. To make things less cluttered, we will use the following standard notation:

$$|+\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \quad |-\rangle := \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

In particular, we observe that

$$H|0\rangle = |+\rangle \quad H|1\rangle = |-\rangle$$

Moreover, we will omit the subscript of the corresponding qubit when the context is clear enough

$$\begin{aligned}
 & q_0 \otimes q_1 \\
 &= |0\rangle \otimes |0\rangle \\
 &\xrightarrow{X(q_1)} |0\rangle \otimes |1\rangle \\
 &\xrightarrow{(H \otimes H)(q_0, q_1)} |+\rangle \otimes |-\rangle \\
 &= \frac{1}{\sqrt{2}}(|00\rangle - |01\rangle + |10\rangle - |11\rangle) \\
 &= \frac{1}{\sqrt{2}}|0\rangle_0 |-\rangle_1 + \frac{1}{\sqrt{2}}|1\rangle_0 |-\rangle_1 \\
 &\xrightarrow{U_f(q_0, q_1)} \frac{1}{\sqrt{2}}(-1)^{f(0)}|0\rangle_0 |-\rangle_1 + \frac{1}{\sqrt{2}}(-1)^{f(1)}|1\rangle_0 |-\rangle_1 \quad (\text{by the lemma}) \\
 &= \frac{1}{\sqrt{2}}((-1)^{f(0)}|0\rangle_0 + (-1)^{f(1)}|1\rangle_0) \otimes |-\rangle_1 \\
 &\xrightarrow{H(q_0)} \frac{1}{\sqrt{2}}((-1)^{f(0)}|+\rangle_0 + (-1)^{f(1)}|-\rangle_0) \otimes \sqrt{2}|-\rangle_1 \\
 &= \frac{1}{2}((-1)^{f(0)}(|0\rangle + |1\rangle) + (-1)^{f(1)}(|0\rangle - |1\rangle)) \otimes \sqrt{2}|-\rangle_1 \\
 &= \frac{1}{2}((((-1)^{f(0)} + (-1)^{f(1)})|0\rangle + ((-1)^{f(0)} - (-1)^{f(1)})|1\rangle) \otimes \sqrt{2}|-\rangle_1
 \end{aligned}$$

Now, since the final operation of the circuit involves measuring $q_0 = \alpha|0\rangle + \beta|1\rangle$, the only two things that we care about are its probability amplitudes, namely

$$\alpha = \frac{1}{2}((-1)^{f(0)} + (-1)^{f(1)})$$

$$\beta = \frac{1}{2} ((-1)^{f(0)} + (-1)^{f(1)})$$

and we see that

- if $f(0) = f(1)$, then

$$(-1)^{f(0)} = (-1)^{f(1)} \implies \begin{cases} \alpha = \frac{1}{2} (2(-1)^{f(0)}) = (-1)^{f(0)} \\ \beta = 0 \end{cases}$$

which implies that

$$q_0 = (-1)^{f(0)} |0\rangle + 0 \cdot |1\rangle = (-1)^{f(0)} |0\rangle$$

and we can ignore the $(-1)^{f(0)}$ factor since its a global phase

- if $f(0) \neq f(1)$, then

$$(-1)^{f(0)} = -(-1)^{f(1)} \implies \begin{cases} \alpha = 0 \\ \beta = \frac{1}{2} (2(-1)^{f(0)}) = (-1)^{f(0)} \end{cases}$$

which implies that

$$q_0 = 0 \cdot |0\rangle + (-1)^{f(0)} |1\rangle = (-1)^{f(0)} |1\rangle$$

by the same reasoning as the other case

In the end, this proves that if $f(0) = f(1)$, q_0 will collapse to $|0\rangle$, while if $f(0) \neq f(1)$, q_1 will collapse to $|1\rangle$, proving that Deutsch's algorithm works correctly.

3.2 Deutsch-Josza algorithm

Even though Deutsch's algorithm is quite interesting and offers advantages that classical computation cannot achieve, still it seems like it wouldn't be very useful in practice. In fact, usually we are interested in the *values* of $f(0)$ and $f(1)$, and as we already mentioned quantum mechanics will not allow us to compute both the values at the same time — meaning that even if we use Deutsch's algorithm to now whether $f(0)$ is equal to $f(1)$ or not, we would still need to compute at least one between $f(0)$ and $f(1)$ in order to know both values.

This is because, in reality, the algorithm that we are using is only solving a particular case of a more complex problem. In fact, a couple of years later Deutsch [Deu92] realized that if we use $q_1 = |1\rangle$ and $q_0 = |0\rangle^{\otimes n}$ (i.e. we use n qubits set to $|0\rangle$) this algorithm is actually able to tell **constant** and **balanced** functions apart.

Definition 3.1: Constant function

A Boolean function $f : \{0, 1\}^n \rightarrow \{0, 1\}$ is said to be **constant** if

$$\exists b \in \{0, 1\} \quad \forall x \in \{0, 1\}^n \quad f(x) = b$$

The definition of constant Boolean function has nothing special, and balanced functions are exactly what the name suggests, i.e. half of the inputs output 0 and the other half output 1, which can be succinctly expressed as follows.

Definition 3.2: Balanced function

A Boolean function $f : \{0, 1\}^n \rightarrow \{0, 1\}$ is said to be **balanced** if it holds that

$$\sum_{x \in \{0,1\}^n} f(x) = 2^{n-1}$$

We observe that a Boolean function can be neither constant nor balanced, so this decision problem is actually a **promise problem**: given a Boolean function f that is either constant or balanced — note that it cannot be both — decide if the function is constant or balanced. Indeed, we see that Deutsch's algorithm solved the same exact problem for $n = 2$: in fact, if $f(0) = f(1)$ it means that f is constant, otherwise the latter is balanced.

Moreover, this problem actually shows the power of quantum parallelism more evidently: with a classical computation, to solve this decision problem we would need at most

$$2^{n-1} + 1 = O(2^n)$$

queries to f , instead our quantum computation still only requires one evaluation of f to solve the problem.

Algorithm 3.2: Deutsch-Josza algorithm

Given a Boolean function f and $n + 1$ qubits, the algorithm returns $|0\rangle^{\otimes n}$ if f is constant, $|1\rangle$ otherwise.

```

1: function DEUTSCHJOSZA( $f, q_0, q_1$ )
2:    $q_1 \leftarrow X(q_1)$ 
3:    $q_0, q_1 \leftarrow (H^{\otimes n} \otimes H)(q_0, q_1)$ 
4:    $q_0, q_1 \leftarrow U_f(q_0, q_1)$ 
5:    $q_0 \leftarrow H^{\otimes n}(q_0)$ 
6:   return measure( $q_0$ )
7: end function
```

Note that in this algorithm q_0 are actually n qubits, thus q_0 is initially set to $|0\rangle^{\otimes n}$. Before proving the correctness of this general version of the algorithm, let us first take a look at the quantum circuit that defines it.

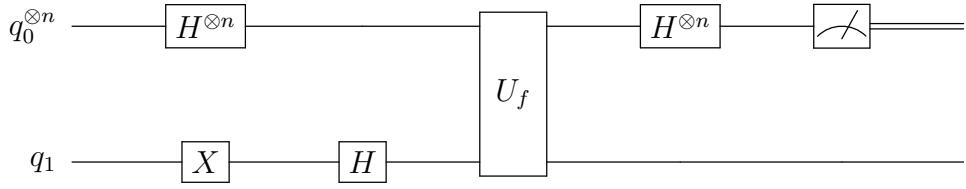


Figure 3.2: The quantum circuit for the Deutsch-Josza algorithm.

Proposition 3.2

For any $x \in \mathbb{B}^n$ it holds that

$$H^{\otimes n} |x\rangle = \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (-1)^{x \cdot a} |a\rangle$$

Proof. First, consider the following claim.

Claim: $\forall a \in \mathbb{B} \quad H|a\rangle = \frac{1}{\sqrt{2}} \sum_{b \in \mathbb{B}} (-1)^{a \cdot b} |b\rangle$.

Proof of the Claim. We observe that

$$H|0\rangle = |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \sum_{b \in \mathbb{B}} (-1)^{0 \cdot b} |b\rangle$$

and analogously

$$H|1\rangle = |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}} \sum_{b \in \mathbb{B}} (-1)^{1 \cdot b} |b\rangle$$

□

In the rest of the proof we will denote with the \cdot symbol the “canonical” scalar product, i.e.

$$\forall x, y \in \mathbb{B}^n \quad x \cdot y := \sum_{i=1}^n x_i y_i$$

Fix $x \in \mathbb{B}^n$; by the previous claim, we have that

$$\begin{aligned} H^{\otimes n} |x\rangle &= \bigotimes_{i=1}^n H|x_i\rangle \\ &= \bigotimes_{i=1}^n \left(\frac{1}{\sqrt{2}} \sum_{b \in \mathbb{B}} (-1)^{x_i b} |b\rangle \right) |x_i\rangle \quad (\text{by the claim}) \\ &= \frac{1}{\sqrt{2^n}} \bigotimes_{i=1}^n (|0\rangle + (-1)^{x_i} |1\rangle) \\ &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (-1)^{x \cdot a} |a\rangle \end{aligned}$$

□

Finally, we are ready to prove the correctness of the algorithm.

$$\begin{aligned}
 & q_0 \otimes q_1 \\
 &= |0\rangle^{\otimes n} \otimes |0\rangle \\
 &\xrightarrow{X(q_1)} |0\rangle^{\otimes n} \otimes |1\rangle \\
 &\xrightarrow{H^{\otimes n}(q_0, q_1)} H^{\otimes n} |0\rangle^{\otimes n} \otimes H |1\rangle \\
 &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (-1)^{0^n \cdot a} |a\rangle \otimes |- \rangle \quad (\text{by Proposition 3.2}) \\
 &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} |a\rangle \otimes |- \rangle \\
 &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (|a\rangle \otimes |- \rangle) \\
 &\xrightarrow{U_f(q_0, q_1)} \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} ((-1)^{f(a)} |a\rangle \otimes |- \rangle) \quad (\text{by Lemma 3.1}) \\
 &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)} |a\rangle \otimes |- \rangle \\
 &\xrightarrow{H^{\otimes n}(q_0)} H^{\otimes n} \left(\frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)} |a\rangle \right) \otimes |- \rangle \\
 &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} ((-1)^{f(a)} H^{\otimes n} |a\rangle) \otimes |- \rangle \\
 &= \frac{1}{\sqrt{2^n}} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)} \left(\frac{1}{\sqrt{2^n}} \sum_{b \in \mathbb{B}^n} (-1)^{a \cdot b} |b\rangle \right) \otimes |- \rangle \quad (\text{by Proposition 3.2}) \\
 &= \frac{1}{2^n} \sum_{a \in \mathbb{B}^n} \sum_{b \in \mathbb{B}^n} (-1)^{f(a)+a \cdot b} |b\rangle \otimes |- \rangle \\
 &= \frac{1}{2^n} \sum_{a \in \mathbb{B}^n} \sum_{b \in \mathbb{B}^n} (-1)^{f(a)+a \cdot b} |b\rangle \otimes |- \rangle \\
 &= \sum_{b \in \mathbb{B}^n} \left(\frac{1}{2^n} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)+a \cdot b} \right) |b\rangle_0 \otimes |- \rangle_1
 \end{aligned}$$

Now note that this state describes the superposition of the system, but the next step of the algorithm will only measure q_0 , therefore we can ignore $|- \rangle_1$ and just focus on the amplitudes of q_0 . Then, by calling

$$\forall b \in \mathbb{B}^n \quad \alpha_b := \frac{1}{2^n} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)+a \cdot b}$$

we can rewrite q_0 as follows

$$q_0 = \sum_{b \in \mathbb{B}^n} \alpha_b |b\rangle$$

Finally, since we want to determine the probability that q_0 collapses into the state $|0\rangle^{\otimes n}$ specifically, we can easily evaluate the associated amplitude of the latter, i.e.

$$\alpha_{0^n} = \frac{1}{2^n} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)+a \cdot 0^n} = \frac{1}{2^n} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)}$$

From this, we can easily conclude that:

- if f is constant, then

$$\alpha_{0^n} = \frac{1}{2^n} \sum_{a \in \mathbb{B}^n} (-1)^{f(a)} = \frac{1}{2^n} \cdot 2^n \cdot (-1)^b = (-1)^b$$

where $b \in \mathbb{B}$, meaning that it is guaranteed that q_0 will collapse to 0^n

- if f is balanced, then

$$\alpha_{0^n} = \frac{1}{2^n} \sum_{a \in \mathbb{B}} (-1)^{f(a)} = \frac{1}{2^n} \cdot 0 = 0$$

meaning that it is guaranteed that q_0 will *not* collapse to 0^n

3.3 Grover's algorithm

Even though Deutsch-Josza algorithm is able to solve the decision problem we described through *one* single evaluation of f , it is fairly apparent that the problem their algorithm solves is quite artificial. However the next algorithm that we are going to discuss solves a problem that is definitely more useful.

In 1996, Grover [Gro97] published a landmark paper called “Quantum Mechanics Helps in Searching for a Needle in a Haystack”, and the name already suggests the problem his work tried to solve: the search problem. The setting is the following: we are given an array of N elements — we can assume that N is always a power of 2 for some n , i.e. $N = 2^n$ — that contains M “solution” elements. However, we do not know their positions, and the problem asks to find the index of any solution element.

More formally, given a Boolean function

$$f : \{0, \dots, N-1\} \rightarrow \mathbb{B} : x \mapsto \begin{cases} 1 & A[x] \in S \\ 0 & \text{otherwise} \end{cases}$$

where A is our array, and S is the set of solution elements, the problem asks to return an x such that $f(x) = 1$, i.e. such that $A[x]$ is a solution.

With a classical computation, it is easy to see that we need $O(\frac{N}{M})$ accesses to A to solve our problem, however we will see that the algorithm Grover developed is able to return a “solution index” in $O(\sqrt{\frac{M}{N}})$ with *high probability*, i.e. Grover's algorithm provides a **quadratic** speedup compared to any classical algorithm — however, it is probabilistic.

Before explaining the details of the algorithm, we need to define some new operators that will be used in Grover's algorithm, and introduce some general notation:

- given an arbitrary qubit $|\psi\rangle$, we will write its superposition of states as follows

$$|\psi\rangle = \sum_{b \in \mathbb{B}^n} \alpha_b |b\rangle$$

where $\sum_{b \in \mathbb{B}^n} |\alpha_b| = 1$

- we define an operator O_f (where f is the indicator function of the array defined before) that computes as follows:

$$\forall x \in \mathbb{B}^n \quad O_f |x\rangle := (-1)^{f(x)} |x\rangle$$

- given an arbitrary qubit $|\psi\rangle$, we define a new operator W as follows:

$$W := 2 |s\rangle \langle s| - I$$

where $|s\rangle$ is the **uniform superposition**, a superposition of states in which each amplitude is equally likely

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{B}^n} |x\rangle$$

- finally, we will define an operator G that will simply compose the last two operators we described

$$G = W \cdot O_f$$

Algorithm 3.3: Grover's algorithm

Given a Boolean function f that describes the solution elements of an array having M solution elements, and n qubits, the algorithm returns a solution index with high probability TODO SPIEGA CHE VUOL DIRE.

```

1: function GROVER( $f, q_0$ )
2:    $q_0 \leftarrow H^{\otimes n}(q_0)$ 
3:   for  $i \in [1, O(\sqrt{\frac{N}{M}})]$  do                                 $\triangleright$  where  $N = 2^n$ 
4:      $q_0 \leftarrow G(q_0)$ 
5:   end for
6:   return measure( $q_0$ )
7: end function

```

First of all, we see that this algorithm takes only n qubits as input, however the actual implementation of the algorithm is slightly different, as shown in the following quantum circuit below.

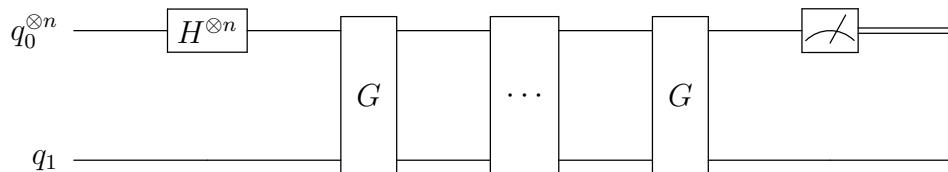


Figure 3.3: The quantum circuit for Grover's algorithm.

Indeed, we can see that the real quantum circuit takes $n + 1$ inputs, and the additional register is called “ancilla” because its only purpose is to actually implement the O_f operator, which is designed exactly as if it was the U_f black-box we discussed in previous algorithms. This can be done thanks to [Lemma 3.1](#), which guarantees that if we give $|-\rangle$ as the second input to U_f we get

$$O_f |x\rangle \otimes |-\rangle = (-1)^{f(x)} \otimes |-\rangle$$

which implies that the ancilla register will still be $|-\rangle$, therefore we can just ignore the second register completely throughout the whole computation, and we are sure that O_f computes correctly.

Furthermore, before proceeding, let us prove that G is actually a unitary operator, i.e. that this is a valid quantum computation.

Claim: The operator G is unitary.

Proof of the Claim. By [Proposition 2.9](#) we know that proving that W and O_f are unitary is sufficient to prove the claim. □

Now that we know this operator is unitary, we can delve into the details of the algorithm. To see what happens at each iteration, we will describe the complete state of the system in a rather unusual way. Let $|a\rangle$ and $|b\rangle$ be the following superpositions:

$$|a\rangle := \frac{1}{\sqrt{N-M}} \sum_{x \in \bar{S}} |x\rangle \quad |b\rangle := \frac{1}{\sqrt{M}} \sum_{x \in S} |x\rangle$$

In other words, $|a\rangle$ is the uniform superposition of non-solution indices, and $|b\rangle$ is the superposition of solution ones. To explain the $\frac{1}{\sqrt{M}}$ factor in front of $|b\rangle$, we recall that in quantum mechanics all state vectors must be normalized, and since the squared norm of $|\tilde{b}\rangle$ (which will denote $|b\rangle$ without the multiplicative factor in front) is equal to

$$\begin{aligned} \langle \tilde{b} | \tilde{b} \rangle &= \left(\sum_{x \in S} |x\rangle \right)^\dagger \left(\sum_{x \in S} |x\rangle \right) \\ &= \left(\sum_{x \in S} \langle x | \right) \left(\sum_{y \in S} |y\rangle \right) \\ &= \sum_{x \in S} \sum_{y \in S} \langle x | y \rangle \\ &= \sum_{x \in S} \sum_{y \in S} \delta_{xy} \quad (\text{basis states are orthonormal}) \\ &= \sum_{x \in S} 1 \\ &= |S| \\ &= M \end{aligned}$$

the norm of $|\tilde{b}\rangle$ is \sqrt{M} , hence to normalize it it suffices to add $\frac{1}{\sqrt{M}}$ in front of $|\tilde{b}\rangle$ —the reasoning for $|a\rangle$ is analogous. Moreover, it's easy to see that $|a\rangle$ and $|b\rangle$ are orthogonal, so they form an orthonormal basis for a 2D space.

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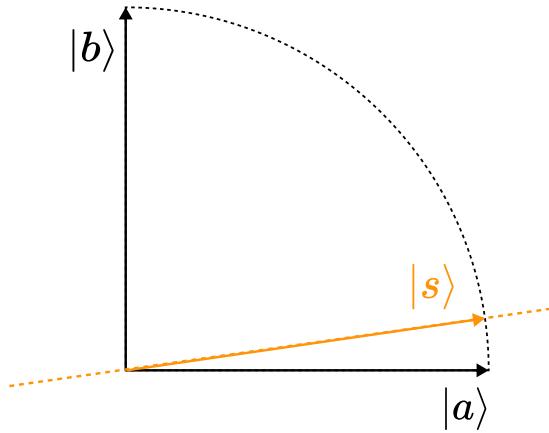
Now, because of how we defined $|a\rangle$ and $|b\rangle$, we can rewrite the uniform superposition

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{B}} |x\rangle$$

as shown below

$$|s\rangle = \sqrt{\frac{N-M}{N}} |a\rangle + \sqrt{\frac{M}{N}} |b\rangle$$

This is quite interesting, because it means that we can describe $|s\rangle$ in terms of $|a\rangle$ and $|b\rangle$. Let us do exactly this, and plot the resulting graph on a 2D space that has $|a\rangle$ and $|b\rangle$ as axis.



We observe that:

- both $|s\rangle$, $|a\rangle$ and $|b\rangle$ are normalized, and all the vectors that we are going to consider are quantum states, so they will be normalized too, therefore we can restrict our focus on a 2D circumference of radius 1 — this plane is usually called **Grover plane**
- since we expect that $M \ll N$, we have that $\sqrt{\frac{M}{N}} \ll \sqrt{\frac{N-M}{N}}$, which basically means that the vector $|s\rangle$ is almost parallel to $|a\rangle$ (the bigger is the number of solution indices, the bigger the angle between $|s\rangle$ and $|a\rangle$)

Consider any state $|\psi\rangle = \sum_{x \in \mathbb{B}^n} \alpha_x |x\rangle$; we observe that

$$\begin{aligned} O_f |\psi\rangle &= O_f \sum_{x \in \mathbb{B}^n} \alpha_x |x\rangle \\ &= \sum_{x \in \mathbb{B}^n} \alpha_x O_f |x\rangle \\ &= \sum_{x \in \mathbb{B}^n} \alpha_x (-1)^{f(x)} |x\rangle \end{aligned}$$

which basically means that each time we apply the O_f operator we are flipping the sign of the amplitudes of the components of $|\psi\rangle$ that represent solution indices. In other words, the O_f operator flips its input w.r.t. $|a\rangle$.

Moreover, we observe that any state $|\psi\rangle$ can be decomposed into

$$|\psi\rangle = \alpha|s\rangle + \beta|\psi_{\perp}\rangle$$

where $\alpha|s\rangle$ is the projection of $|\psi\rangle$ along $|s\rangle$'s space — thus $\alpha = \langle s|\psi\rangle$ — and $|\psi_{\perp}\rangle$ is the projection of $|\psi\rangle$ along the space that is orthogonal to $|s\rangle$'s. Therefore, we have that

$$\begin{aligned} W|\psi\rangle &= W(\alpha|s\rangle + \beta|\psi_{\perp}\rangle) \\ &= 2|s\rangle\langle s|(\alpha|s\rangle + \beta|\psi_{\perp}\rangle) - (\alpha|s\rangle + \beta|\psi_{\perp}\rangle) \\ &= 2\alpha|s\rangle\langle s|s\rangle + 2\beta|s\rangle\langle s|\psi_{\perp}\rangle - (\alpha|s\rangle + \beta|\psi_{\perp}\rangle) \\ &= 2\alpha|s\rangle \cdot 1 + 0 - (\alpha|s\rangle + \beta|\psi_{\perp}\rangle) \\ &= \alpha|s\rangle - \beta|\psi_{\perp}\rangle \end{aligned}$$

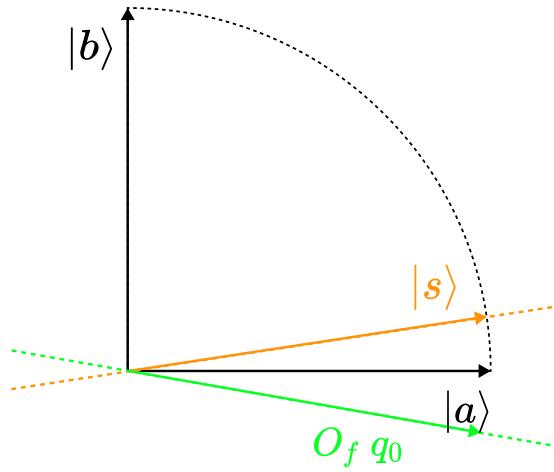
which means that what W actually performs is leaving the component along $|s\rangle$'s space unchanged, and it flips the sign of the component of the orthogonal space. In other words, what W computes is the reflection of $|\psi\rangle$ w.r.t. $|s\rangle$.

We can finally describe Grover's algorithm in detail. First, we see that

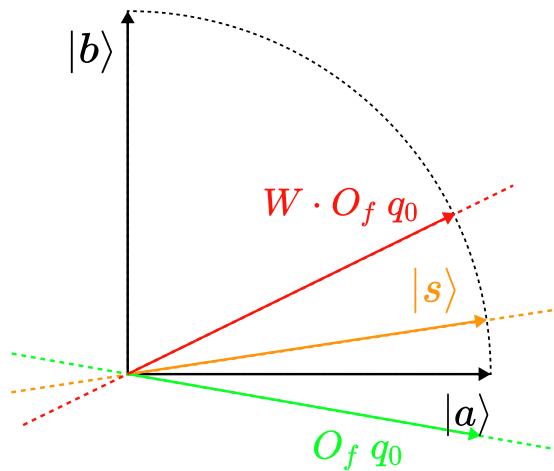
$$\begin{aligned} q_0 &= |0\rangle^{\otimes n} \\ &\xrightarrow{H^{\otimes n}(q_0)} \frac{1}{\sqrt{2^n}} \sum_{x \in \mathbb{B}^n} (-1)^{0^n \cdot x} |x\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{B}^n} |x\rangle \\ &= |s\rangle \end{aligned}$$

Indeed, the only purpose of the first Hadamard operator is to “move” the initial state slightly away from $|a\rangle$ — and also making each component initially equally likely. Now, let's see what happens at each application of the $G = W \cdot O_f$ operator:

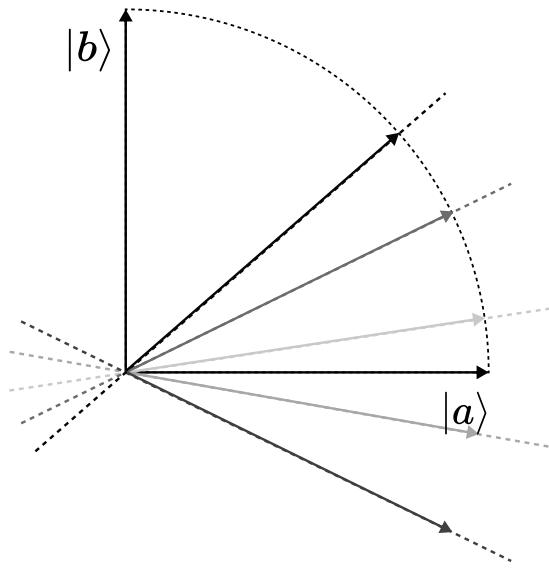
- as previously shown, the operator O_f reflects its input w.r.t. the $|a\rangle$ axis — below we show what happens when we first apply O_f $q_0 = O_f|s\rangle$:



- additionally, as previously explained the operator W reflects its input w.r.t. the axis described by the $|s\rangle$ vector, thus when we compute $W \cdot O_f q_0$ we will end up with the following vector:



- this suggests that each time we apply the operator G we are making q_0 closer and closer to $|b\rangle$, as depicted below:



This is the core idea of Grover's algorithm: if we rewrite q_0 in terms of $|a\rangle$ and $|b\rangle$

$$q_0 = \beta_0 |a\rangle + \beta_1 |b\rangle$$

we get that through Grover's algorithm we transformed q_0 such that it is now very close to $|b\rangle$, meaning that $\beta_0 \ll \beta_1$. This directly implies that when we will measure q_0 at the end of Grover's procedure the likelihood that it will collapse into some $|x\rangle$ that is a component of $|b\rangle$ — i.e. a solution index — is very high. In other words, what happens with Grover's algorithm is that we gradually increase the amplitudes of the solution indices, in order to maximize the probability that our qubit will collapse in one them when it will be measured at the end of the procedure.

Now that we know how Grover's algorithm works, the only thing left to discuss is the $O\left(\sqrt{\frac{N}{M}}\right)$ factor. Why is it guaranteed that after this amount of applications of the G operator we are done with the algorithm? Well, we actually have the opposite problem: in reality, we have to *stop early enough*. Consider again how Grover's algorithm operates in the Grover plane; clearly, if we apply G too many times, what happens is that q_0 will end up past $|b\rangle$ itself:

Let the angle between $|a\rangle$ and $|s\rangle$ be θ ; since O_f flips q_0 w.r.t. $|a\rangle$, and W flips $O_f q_0$ w.r.t. $|s\rangle$, G will cumulatively rotate q_0 by 2θ : [More formally, we can actually show that](#)

[drawing](#)

[drawing](#)

Proposition 3.3

The Grover operator G can be rewritten in the basis $\{|a\rangle, |b\rangle\}$ as follows:

$$G = \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix}$$

where $|s\rangle = \cos \theta |a\rangle + \sin \theta |b\rangle$.

Proof. First, we need two small identities in trigonometry.

Claim 1: For any angle θ it holds that $2\cos^2 \theta - 1 = \cos 2\theta$.

Proof of the Claim. Through algebraic manipulation we have that

$$\begin{aligned} 2\cos^2 \theta - 1 &= 2\cos^2 \theta - (\sin^2 \theta + \cos^2 \theta) \\ &= 2\cos^2 \theta - \sin^2 \theta - \cos^2 \theta \\ &= \cos^2 \theta - \sin^2 \theta \\ &= \cos 2\theta \quad (\text{double-angle formula}) \end{aligned}$$

□

Claim 2: For any angle θ it holds that $1 - 2\sin^2 \theta = \cos 2\theta$.

Proof of the Claim. From the previous claim we have that

$$1 - 2\sin^2 \theta = 1 - 2(1 - \cos^2 \theta) = 1 - 2 + 2\cos^2 \theta = 1 + \cos 2\theta - 1 = \cos 2\theta$$

□

Let $|v\rangle$ be any vector described inside the $\{|a\rangle, |b\rangle\}$:

$$|v\rangle = \alpha |a\rangle + \beta |b\rangle$$

We already saw how the O_f operator flips its input w.r.t. the $|a\rangle$ axis, indeed its action on $|v\rangle$ would be the following:

$$O_f |v\rangle = \alpha |a\rangle - \beta |b\rangle$$

Thus, starting from the definition of G , by the two previous claims we have that

$$\begin{aligned}
 G|v\rangle &= W \cdot O_f|v\rangle \\
 &= W \cdot (\alpha|a\rangle - \beta|b\rangle) \\
 &= (2|s\rangle\langle s| - I)(\alpha|a\rangle - \beta|b\rangle) \\
 &= 2|s\rangle\langle s|(\alpha|a\rangle - \beta|b\rangle) - (\alpha|a\rangle - \beta|b\rangle) \\
 &= 2|s\rangle(\cos\theta|a\rangle + \sin\theta|b\rangle)^\dagger(\alpha|a\rangle - \beta|b\rangle) - (\alpha|a\rangle - \beta|b\rangle) \\
 &= 2|s\rangle(\cos\theta\langle a| + \sin\theta\langle b|)(\alpha|a\rangle - \beta|b\rangle) - (\alpha|a\rangle - \beta|b\rangle) \\
 &= 2|s\rangle(\alpha\cos\theta - \beta\sin\theta) - (\alpha|a\rangle - \beta|b\rangle) \\
 &= 2(\cos\theta|a\rangle + \sin\theta|b\rangle)(\alpha\cos\theta - \beta\sin\theta) - (\alpha|a\rangle - \beta|b\rangle) \\
 &= 2\alpha\cos^2\theta|a\rangle - 2\beta\cos\theta\sin\theta|a\rangle + 2\alpha\sin\theta\cos\theta|b\rangle - 2\beta\sin^2\theta|b\rangle - \alpha|a\rangle + \beta|b\rangle \\
 &= [\alpha(2\cos^2\theta - 1) - 2\beta\cos\theta\sin\theta]|a\rangle + [\beta(1 - 2\sin^2\theta) + 2\alpha\sin\theta\cos\theta]|b\rangle \\
 &= (\alpha\cos 2\theta - \beta\sin 2\theta)|a\rangle + (\alpha\sin 2\theta + \beta\cos 2\theta)|b\rangle \\
 &= \begin{pmatrix} \alpha\cos 2\theta - \beta\sin 2\theta \\ \alpha\sin 2\theta + \beta\cos 2\theta \end{pmatrix} \\
 &= \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\
 &= \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix}|v\rangle
 \end{aligned}$$

which concludes that G must be the rotation matrix of 2θ . \square

Indeed, with each application of G we are rotating q_0 by 2θ , which means that at the k -th application it holds that

$$G^k q_0 = \cos((2k+1)\theta)|a\rangle + \sin((2k+1)\theta)|b\rangle$$

for any $k \in \mathbb{N}$, where the additional 1 comes from the fact that $q_0 = |s\rangle$ through the Hadamard transformation at the start of the process. Thus, to evaluate the optimal number of iterations we need to find the optimal k , i.e. the one that maximizes the probability of measuring a solution index, which is equal to the squared amplitude of $|b\rangle$, namely

$$\Pr[\text{measure}(q_0) = |b\rangle] = \sin^2((2k+1)\theta)$$

Hence, we have that $\sin^2((2k+1)\theta) = 1$ when $(2k+1)\theta = \frac{\pi}{2}$, and solving for k we get that

$$k = \frac{\pi}{4\theta} - \frac{1}{2}$$

Lastly, since θ is the angle between $|a\rangle$ and $|s\rangle$, we can rewrite $|s\rangle$ as

$$|s\rangle = \cos\theta|a\rangle + \sin\theta|b\rangle$$

which directly implies that

$$\sin\theta = \sqrt{\frac{M}{N}} \iff \theta = \arcsin\sqrt{\frac{M}{N}}$$

and therefore

$$\begin{aligned}
k &= \frac{\pi}{4\theta} - \frac{1}{2} \\
&= \frac{\pi}{4 \arcsin \sqrt{\frac{M}{N}}} - \frac{1}{2} \\
&\leq \frac{\pi}{4 \arcsin \sqrt{\frac{M}{N}}} \\
&\leq \frac{\pi}{4 \sqrt{\frac{M}{N}}} \\
&= \frac{\pi}{4} \sqrt{\frac{N}{M}} \\
&= O\left(\sqrt{\frac{N}{M}}\right)
\end{aligned}$$

which finally explains the quadratic speedup of Grover's algorithm w.r.t. the classical version of the problem.

As a final note, we observe that Grover's algorithm assumes that $\theta \leq \frac{\pi}{4}$, otherwise we overshoot $|b\rangle$ with a single iteration of the G operator — since $\theta > \frac{\pi}{4}$ would mean that $|s\rangle$ is placed on the “upper half” of the Grover plane. However, to ensure this constraint on θ we only need that $M \leq \frac{N}{2}$, i.e. at most half of the elements in our array are solution elements. Indeed, we see that

$$M \leq \frac{N}{2} \implies \sin \theta = \sqrt{\frac{M}{N}} \leq \sqrt{\frac{1}{2}} \implies \theta \leq \arcsin \sqrt{\frac{1}{2}} = \frac{\pi}{4}$$

What can we do if the number of solutions is more than half the size of the array? We simply invert the problem and find the non-solutions!

3.3.1 Another perspective

Interestingly enough, we can look at what happens to the amplitudes of q_0 from another perspective. Usually, the W operator is called **diffusion operator**, and what it does is computing the so called *inversion about the mean* of its input. Consider any state

$|\psi\rangle = \sum_{x \in \mathbb{B}^n} \alpha_x |x\rangle$, and observe that

$$\begin{aligned}
 \langle s | \psi \rangle &= \left(\frac{1}{\sqrt{N}} \sum_{y \in \mathbb{B}^n} |y\rangle \right)^\dagger \left(\sum_{x \in \mathbb{B}^n} \alpha_x |x\rangle \right) && (\text{since } \langle s | = |s\rangle^\dagger) \\
 &= \left(\frac{1}{\sqrt{N}} \sum_{y \in \mathbb{B}^n} \langle y | \right) \left(\sum_{x \in \mathbb{B}^n} \alpha_x |x\rangle \right) \\
 &= \frac{1}{\sqrt{N}} \sum_{y \in \mathbb{B}^n} \sum_{x \in \mathbb{B}^n} \alpha_x \langle y | x \rangle \\
 &= \frac{1}{\sqrt{N}} \sum_{y \in \mathbb{B}^n} \sum_{x \in \mathbb{B}^n} \alpha_x \delta_{xy} && (\text{basis states are orthonormal}) \\
 &= \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{B}^n} \alpha_x \sum_{y \in \mathbb{B}^n} \delta_{xy} \\
 &= \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{B}^n} \alpha_x \\
 &= \sqrt{N} \bar{\alpha}_\psi
 \end{aligned}$$

where $\bar{\alpha}_\psi$ is the average amplitude of $|\psi\rangle$. This implies that

$$\begin{aligned}
 W |\psi\rangle &= (2|s\rangle\langle s| - I) |\psi\rangle \\
 &= 2|s\rangle\langle s|\psi\rangle - \sum_{x \in \mathbb{B}^n} |x\rangle \\
 &= 2|s\rangle \left(\sqrt{N} \bar{\alpha}_\psi \right) - \sum_{x \in \alpha_x |x\rangle} && (\text{for the previous observation}) \\
 &= 2 \left(\frac{1}{\sqrt{N}} \sum_{y \in \mathbb{B}^n} |y\rangle \right) \sqrt{N} \bar{\alpha}_\psi - \sum_{x \in \mathbb{B}^n} \alpha_x |x\rangle \\
 &= \sum_{x \in \mathbb{B}^n} (2\bar{\alpha}_\psi - \alpha_x) |x\rangle
 \end{aligned}$$

In other words, when we apply W to a superposition of states, what happens is that each amplitude of the basis states is trasformed as follows:

$$W : \alpha_x \rightarrow 2\bar{\alpha}_\psi - \alpha_x$$

To understand why this is important, let's look at what happens in Grover's algorithm after the first Hadamard application. TODO

da finire

3.3.2 Fixed-Point Quantum Search

As we saw in the previous sections, with Grover's algorithm we need to be careful on how many times we apply the G operator, however we observe that the right value for k — i.e. the number of iterations — strictly depends on both N and M . Assuming that N , the length of the array, is known, it is not guaranteed that we know M too (the number of

solutions in the array). Therefore, if we want to apply Grover's algorithm we also need to be able to to a rough estimate on M , otherwise we might end up stopping either too early or too late. This makes Grover's algorithm fragile in some real-world scenarios.

Grover was actually aware of this problem, and in 2005 he designed a new algorithm which is able to solve this issue [Gro05]. The idea of the algorithm is to *monotonically* increase the probability of finding a solution, without oscillating back down $|a\rangle$. This algorithm is called **Fixed-Point Quantum Search**, because the solutions actually become a “stable fixed point” of the transformation — i.e. once you reach a good solution, further iterations leave it basically unchanged. Indeed, with Grover's search each iteration is a constant-angle rotation, while in fixed-point search we will see that the phase angles in each rotation changes such that the rotation angle decreases over time.

First, we need to define two new operators:

$$R_s := I - (1 - e^{i\theta}) |s\rangle \langle s| \quad R_t := I - (1 - e^{i\theta}) |t\rangle \langle t|$$

where $|s\rangle$ is the starting state and $|t\rangle$ is the target state (in Grover's algorithm this was $|b\rangle$) — this is the original notation that Grover used in his paper, and actually explains why we used $|s\rangle$ in the previous version of the algorithm, it's just the “start”. These two operators are called **phase shift operators**; as usual, before proceeding we need to show that both operators are actually unitary.

Claim: R_t and R_s are unitary operators.

Proof of the Claim. TODO



What are these two operators in the first place? When we presented the W operator, we also noticed how it actually performs a reflection of its input w.r.t. the space of $|s\rangle$. Well, through a very similar argument it can be shown that

$$W^\perp := I - 2|s\rangle \langle s|$$

performs a reflection of its input w.r.t. the space *orthogonal* to $|s\rangle$ — indeed, we end up with

$$W^\perp |\psi\rangle = \beta |\psi_\perp\rangle - \alpha |s\rangle$$

If we now look at the R_s operator, we can see that when we actually compute the reflection it performs we end up with

$$R_s |\psi\rangle = \beta |\psi_\perp\rangle + e^{i\theta} \alpha |s\rangle$$

This suggests that what R_s actually computes is a “soft reflection” w.r.t. the space perpendicular to $|s\rangle$. Through an analogous argument, we can see that

$$R_t |\psi\rangle = \beta |\psi_\perp\rangle + e^{i\theta} \alpha |t\rangle$$

meaning that R_t computes a “soft reflection” w.r.t. the space perpendicular to $|t\rangle$ — however, we observe that the latter is literally the space of $|a\rangle$, indeed O in Grover's algorithm could have been defined as

$$O = I - 2|b\rangle \langle b|$$

and indeed it is sometimes defined such.

Now, we are going to define an addition operator called U as such: let U be any unitary operator such that, for some small $\varepsilon > 0$, it holds that

$$|\langle t|Us\rangle|^2 = 1 - \varepsilon$$

We observe that

- by the laws of quantum mechanics we have that

$$\Pr[\text{measure}(U|s\rangle) = |t\rangle] = |\langle t|Us\rangle|^2$$

therefore we require U to be an operator such that it “drives $|s\rangle$ close to $|t\rangle$ with high probability” — i.e. $1 - \varepsilon$

- we know that U exists since it's just a rotation in a 2D space
- also, a geometric interpretation of the scalar product is that we are measuring the cosine of the angle between $|t\rangle$ and $|Us\rangle$, and we want this value to be very high (such that the angle would be very small) — we observe that we are in Hilbert spaces so the notion of “angle” is not the same of the one we are used to with Euclidean spaces, but this is just to have an idea of what is happening with U

Moreover, define the following operator

$$G := UR_s U^\dagger R_t U$$

Let's see what happens when we evaluate $G|s\rangle$. By denoting $U_{ts} = \langle t|Us\rangle$, we can prove the following equality.

Lemma 3.2

It holds that

$$G|s\rangle = U|s\rangle \left[e^{i\theta} + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right] + |t\rangle U_{ts} (e^{i\theta} - 1)$$

Proof. First, we prove the following equality.

Claim: It holds that $\langle s|U^\dagger|t\rangle U_{ts} = |U_{ts}|^2$.

Proof of the Claim.

$$\begin{aligned} \langle s|U^\dagger|t\rangle U_{ts} &= \langle s|U^\dagger t\rangle U_{ts} \\ &= \langle Us|t\rangle U_{ts} && (\text{by def. of adjoint}) \\ &= \overline{\langle t|Us\rangle} U_{ts} && (\text{by prop. of scalar products}) \\ &= \overline{U_{ts}} U_{ts} \\ &= |U_{ts}|^2 && (z \cdot \bar{z} = |z|^2) \end{aligned}$$

□

Let $P_s = |s\rangle\langle s|$ and $P_t = |t\rangle\langle t|$; thus, we have that

$$\begin{aligned}
 G &= UR_sU^\dagger R_t U \\
 &= U(I - (1 - e^{i\theta})P_s)U^\dagger(I - (1 - e^{i\theta})P_t)U \\
 &= (U - (1 - e^{i\theta})UP_s)U^\dagger(U - (1 - e^{i\theta})UP_t) \\
 &= (UU^\dagger - (1 - e^{i\theta})UP_sU^\dagger)(U - (1 - e^{i\theta})UP_t) \\
 &= (I - (1 - e^{i\theta})UP_sU^\dagger)(U - (1 - e^{i\theta})UP_t) \quad (UU^\dagger = I) \\
 &= U - (1 - e^{i\theta})P_tU - (1 - e^{i\theta})UP_s + (1 - e^{i\theta})^2UP_sU^\dagger P_tU
 \end{aligned}$$

Therefore, we find that $G|s\rangle$ can be evaluated as follows:

$$\begin{aligned}
 G|s\rangle &= (U - (1 - e^{i\theta})P_tU - (1 - e^{i\theta})UP_s + (1 - e^{i\theta})UP_sU^\dagger P_tU)|s\rangle \\
 &= U|s\rangle - (1 - e^{i\theta})P_tU|s\rangle - (1 - e^{i\theta})UP_s|s\rangle + (1 - e^{i\theta})^2UP_sU^\dagger P_tU|s\rangle \\
 &= U|s\rangle - (1 - e^{i\theta})|t\rangle U_{ts} - (1 - e^{i\theta})U|s\rangle + (1 - e^{i\theta})^2U|s\rangle\langle s|U^\dagger|t\rangle U_{ts} \\
 &= U|s\rangle - (1 - e^{i\theta})|t\rangle U_{ts} - (1 - e^{i\theta})U|s\rangle + (1 - e^{i\theta})^2U|s\rangle|U_{ts}|^2 \quad (\text{by the claim}) \\
 &= \dots \quad (\text{algebraic manipulation}) \\
 &= U|s\rangle \left[e^{i\theta} + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right] + |t\rangle U_{ts} (e^{i\theta} - 1)
 \end{aligned}$$

□

Most importantly, this equality can be used in the following proposition, which shows that we can actually find an angle θ for which the distance from $|t\rangle$ decreases significantly.

Proposition 3.4

There exists an angle θ such that

$$\Pr[\text{measure}(G|s\rangle) = |t\rangle] = 1 - \varepsilon^3$$

Proof. Thanks to the previous lemma, we obtain that

$$\begin{aligned}
 \Pr[\text{measure}(G|s\rangle) = |t\rangle] &= |\langle t|G_s\rangle|^2 \\
 &= \left| \langle t| \left[U|s\rangle \left(e^{i\theta} + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right) + |t\rangle U_{ts} (e^{i\theta} - 1) \right] \right|^2 \\
 &= \left| \langle t|U_s\rangle \left(e^{i\theta} + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right) + \langle t|t\rangle U_{ts} (e^{i\theta} - 1) \right|^2 \\
 &= \left| U_{ts} \left(e^{i\theta} + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right) + U_{ts} (e^{i\theta} - 1) \right|^2 \\
 &= \left| U_{ts} \left[2e^{i\theta} - 1 + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right] \right|^2 \\
 &= |U_{ts}|^2 \cdot \left| 2e^{i\theta} - 1 + |U_{ts}|^2 (e^{i\theta} - 1)^2 \right|^2 \\
 &= (1 - \varepsilon) \cdot \left| 2e^{i\theta} - 1 + (1 - \varepsilon) (e^{i\theta} - 1)^2 \right|^2 \quad (|U_{ts}|^2 = 1 - \varepsilon)
 \end{aligned}$$

Now, let's see what happens if we set $\theta = \frac{\pi}{3}$: we obtain that

$$\begin{aligned}
 \Pr[\text{measure}(G|s\rangle) = |t\rangle] &= (1 - \varepsilon) \cdot \left| 2e^{i\frac{\pi}{3}} - 1 + (1 - \varepsilon) \left(e^{i\frac{\pi}{3}} - 1 \right)^2 \right|^2 \\
 &= (1 - \varepsilon) \cdot \left| 2e^{i\frac{\pi}{3}} - 1 - (1 - \varepsilon)i\frac{\pi}{3} \right|^2 \quad \left(\left(e^{i\frac{\pi}{3}} - 1 \right)^2 = -e^{i\frac{\pi}{3}} \right) \\
 &= (1 - \varepsilon) \cdot \left| (1 + \varepsilon)e^{i\frac{\pi}{3}} - 1 \right|^2 \\
 &= (1 - \varepsilon) \cdot \left| (1 + \varepsilon) \left(\frac{1}{2} + i\frac{\sqrt{4}}{2} \right) - 1 \right|^2 \quad (\text{by Euler's formula}) \\
 &= (1 - \varepsilon) \cdot \left| \frac{1}{2} + i\frac{\sqrt{3}}{2} + \frac{\varepsilon}{2} + i\frac{\sqrt{3}}{2}\varepsilon - 1 \right|^2 \\
 &= (1 - \varepsilon) \cdot \left| \frac{\varepsilon}{2} - \frac{1}{2} + i\frac{\sqrt{3}}{2}(1 + \varepsilon) \right|^2 \\
 &= (1 - \varepsilon) \cdot \left[\left(\frac{\varepsilon}{2} - \frac{1}{2} \right)^2 + \left(\frac{\sqrt{3}}{2}(1 + \varepsilon) \right)^2 \right] \quad (|z|^2 = \Re^2(z) + \Im^2(z)) \\
 &= (1 - \varepsilon) \cdot (1 + \varepsilon + \varepsilon^2) \\
 &= 1 + \varepsilon + \varepsilon^2 - \varepsilon - \varepsilon^2 - \varepsilon^3 \\
 &= 1 - \varepsilon^3
 \end{aligned}$$

This shows that by applying G the probability of measuring $|t\rangle$ has increased from $1 - \varepsilon$ to $1 - \varepsilon^3$. \square

Indeed, it can be shown that by defining the following recursive sequence of operators

$$\begin{cases} U_0 := U & m = 0 \\ U_m = U_{m-1} R_s U_{m-1}^\dagger R_t U_{m-1} & m \geq 1 \end{cases}$$

we get that

$$\Pr[\text{measure}(|U_m\rangle|s\rangle) = |t\rangle] = \langle \langle t | U_m s \rangle \rangle^2 = 1 - \varepsilon^{2q_m+1}$$

where q_m is the number of queries of $f(x)$.

TODO

Unfortunately, there already exists a classical probabilistic algorithm that the failure probability drops as ε^{q+1} after q queries to f . Thus, the quantum advantage with this method is lost.

So, what do we do now? In 2014 Yoder, Low, and Chuang [YLC14] proposed a fixed-point quantum search algorithm that monotonically converges to the target state while still retaining the quadratic advantage of the original Grover's algorithm over classical algorithms. The algorithm involves phase-shift operators that are parametrized with angles different from $\theta = \frac{\pi}{3}$, and again involves building a sequence of operators using

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said phase shifts. However, the details of this result are way beyond the scope of our discussion, so we won't describe the details of their findings.

4

Quantum Phase Estimation

Shor's algorithm is a quantum algorithm for finding the *prime factors of an integer*, developed in 1994 by the American mathematician Shor [Sho]. It is one of the few known quantum algorithms with compelling potential applications and strong evidence of **superpolynomial** speedup compared to best known classical (non-quantum) algorithm. It is one of the most famous algorithms in the field, and it sparked a lot of interest in recent years due to the implications of its theoretical speedup.

Shor's algorithm utilizes a lot of mathematical tools

Before explaining Shor's algorithm, we first need to present a very useful tool that is widely employed in various areas of computer science and mathematics, such as integer multiplication, signal processing (e.g. speech recognition, audio compression) and much more.

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4.1 A recap on the Discrete Fourier Transform

The **Discrete Fourier Transform (DFT)** is a very powerful tool used in many applications and probably most widely known for its use in signal processing. Indeed, the Fourier transform is used to transform a signal defined on the *time domain* into its equivalent in the *frequency domain*. We will briefly explore the most important concepts that define the DFT to have a better understanding in order to the progress with its quantum counterpart.

First, what is the “time domain”? When we sample a signal, we usually sample such signal through some finite amount of time, and we discretize such time interval — this is why we consider the Discrete Fourier transform. What we are interested in is to transform such signal into the “frequency domain”, which essentially means to understand what frequencies of sinusoids contribute to our signal and in which percentage. To do this, we will use some concepts of Linear Algebra. Say that the signal we sampled is discretized into N parts, thus our sample lives in the \mathbb{R}^N space — it is nothing but a vector of N complex values which describe the signal at each timestep. When we say “time domain”,

what we mean is basically this exact vector, i.e. expressed in the canonical orthonormal basis

$$e_0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad e_1 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} \quad \dots \quad e_{N-1} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

(we will start counting at 0 for convenience sake). In other words, if our signal is defined by some vector

$$\mathbf{x} = \begin{pmatrix} t_0 \\ t_1 \\ \vdots \\ t_{N-1} \end{pmatrix}$$

it holds that

$$\mathbf{x} = \sum_{n=0}^{N-1} t_n e_n$$

Then, what is the “frequency domain”? We need some preliminary observations to describe it. Our goal is to take into account the frequencies that define our signal, therefore we need to move into a space in which frequencies are “first-class citizens”. The idea is to use each possible sinusoid by varying the frequency, add up their contributions, and weight the latter in the precise way that allows us to reconstruct our original signal. Let us fix a component $n \in [0, N - 1]$, and first consider only cosinusoids, for instance

$$\cos(2\pi \cdot 0 \cdot n) \quad \cos(2\pi \cdot 1 \cdot n) \quad \cos(2\pi \cdot 2 \cdot n) \quad \dots \quad \cos(2\pi \cdot (N - 1) \cdot n)$$

Basically, we are trying to construct a basis built on each possible frequency f by obtaining a basis vector $\cos(2\pi \cdot f \cdot n)$. Moreover, we will consider $\cos(2\pi m n / N)$ for $m \in [0, N - 1]$ since it can be shown that the number of possible frequencies that can be represented on a N -sized time window is exactly N , and to scale the frequency accordingly we just need to divide m over N , the size of the sample.

Is this enough to reach our goal? Can we describe any signal in this way? Well, we observe that m is ranging from 0 to $N - 1$, but $\cos(-\theta) = \cos(\theta)$, which implies that

$$m > \frac{N}{2} \implies \cos(2\pi m n / N) = \cos(2\pi(N - m)n / N)$$

In other words, basically half of our basis vectors add no information at all. Indeed, the span of the vectors we chose has size

$$\dim \left(\text{span} \left(\{\cos(2\pi \cdot m \cdot n / N)\}_{m=1}^{N-1} \right) \right) = \begin{cases} \frac{N}{2} + 1 & N \text{ is even} \\ \frac{N+1}{2} & N \text{ is odd} \end{cases}$$

where the last added 1 comes from the fact that when $m = 0$ we generate $\cos(0) = 1$ which is really linearly independent from the others cosines. This suggests that cosinusoids alone are not enough to describe our space.

Hence, the most natural thing that we can do is add the contributions of sinusoids as well. A geometric interpretation of the fact that cosinusoids are not enough is that sinusoids are just phase-shifted cosines, but the shift in phase is not captured by changing the frequencies of the cosines alone. We need the contributions of some “altered” cosinusoids — in terms of phases — to get an actual basis and be able to represent any possible vector. Hence, let’s consider additional N sinusoids

$$\sin(2\pi \cdot 0 \cdot n) \quad \sin(2\pi \cdot 1 \cdot n) \quad \sin(2\pi \cdot 2 \cdot n) \quad \dots \quad \sin(2\pi \cdot (N-1) \cdot n)$$

Do we get a base of size more than N then? We observe that $\sin(\theta) = -\sin(-\theta)$, therefore we have that

$$m > \frac{N}{2} \implies \sin(2\pi mn/N) = -\sin(2\pi(N-m)n/N)$$

which again it implies that half of these sinusoids add no useful information. However, in this case we also have the fact that

$$\sin(2\pi \cdot 0 \cdot n/M) = \sin(0) = 0$$

and for N even it also happens that

$$\sin(2\pi \cdot (N/2) \cdot n/N) = \sin(\pi n) = 0$$

which means that these two sinusoid cannot be considered because they are the 0 vector of this space. Therefore, we get that

$$\dim \left(\text{span} \left(\{\sin(2\pi \cdot m \cdot n/N)\}_{m=1}^{N-1} \right) \right) = \begin{cases} \frac{N}{2} - 1 & N \text{ is even} \\ \frac{N-1}{2} & N \text{ is odd} \end{cases}$$

Finally, this means that putting all these cosines and sinusoids together we form a base for a space that has size

$$\begin{cases} \frac{N}{2} + 1 + \frac{N}{2} - 1 = N & N \text{ is even} \\ \frac{N+1}{2} + \frac{N-1}{2} = N & N \text{ is odd} \end{cases} = N$$

Hence, we can fully describe \mathbb{R}^N , namely for any vector $\mathbf{x} \in \mathbb{R}^N$ we have that

$$\forall n \in [0, N-1] \quad \mathbf{x}(n) = \sum_{m=0}^{N-1} \alpha_m \cos(2\pi mn/N) + \sum_{m=0}^{N-1} \beta_m \sin(2\pi mn/N)$$

by describing the vector component-wise.

Furthermore, we observe that this basis is actually orthogonal.

Now, the last thing that we need to do is move into the complex space \mathbb{C}^N . Thankfully, we can leverage the very powerful Euler’s formula

$$e^{i\theta} = \cos \theta + i \sin \theta$$

to immediately sum the contributions of cosinusoids and sinusoids into a single value $e^{2\pi imn/N}$. In other words, for any vector $\mathbf{x} \in \mathbb{C}^N$ it holds that

$$\forall n \in [0, N-1] \quad \mathbf{x}(n) = \sum_{m=0}^{N-1} \gamma_m e^{2\pi imn/N}$$

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The basis of this space is thus

$$e^{2\pi i \cdot 0 \cdot x/N} \quad e^{2\pi i \cdot 1 \cdot x/N} \quad \dots \quad e^{2\pi i \cdot (N-1) \cdot x/N}$$

We observe that this basis is orthogonal as well, but it's not orthonormal in fact Hence, because the norm of each vector is

$$\begin{aligned} \sqrt{\langle e^{2\pi imn/N} | e^{2\pi imn/N} \rangle} &= \sqrt{\sum_{n=0}^{N-1} e^{2\pi imn/N} \cdot \overline{e^{2\pi imn/N}}} \\ &= \sqrt{\sum_{n=0}^{N-1} |e^{2\pi imn/N}|^2} \\ &= \sqrt{\sum_{n=0}^{N-1} 1} \\ &= \sqrt{N} \end{aligned}$$

we usually consider the same base but scaled by a factor of $\frac{1}{\sqrt{N}}$, i.e.

$$\forall n \in [0, N-1] \quad \mathbf{x}(n) = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} \delta_m e^{2\pi imn/N}$$

We define δ_m to be the m -th component of the **discrete Fourier transform** of \mathbf{x} , and the operation that reconstructs $\mathbf{x}(n)$ is called **inverse discrete Fourier transform**. In other words, the DFT of a vector computes the projection of said vector into the space \mathbb{C}^N through the orthonormal basis

$$\left\{ \frac{1}{\sqrt{N}} e^{2\pi imn/N} \right\}_{m=0}^{N-1}$$

Indeed, we can compute the DFT by simply applying the matrix that performs the **change of basis**, but we will see the details of this idea in the next section.

4.2 The Quantum Fourier Transform

Now that we have a general understanding of what the DFT is, let's see how the matrix operation is actually defined.

Definition 4.1: n -th root of unity

Given a commutative ring R , and a natural number $n \in N$, an element $\omega \in R$ is called **n -th root of unity** if $\omega^n = 1$.

For instance, $-i$ is a 4-th root of unity, in fact $(-i)^4 = 1$. We observe that, since multiplication in the complex plane is a rotation, the n -th roots of 1 evenly divide the unit circle as shown below:

TODO

drawing

Now, among all possible n -th roots of unity we are going to provide a more specific definition. Let the **order of an n -th root of unity** ω be the smallest power d such that $\omega^d = 1$. For instance, $(-1)^4 = 1$ indeed -1 is a 4-th root of unity, however its order is 2 since $(-1)^2 = 1$ and $2 < 4$.

Definition 4.2: Principal n -th root of unity

Given an n -th root of unity ω , we say that ω is **principal** if and only if $\omega \neq 1$ and the order of ω is n .

In other words, the principal n -th root of unity is the first root (after 1) that we encounter on the unit circle. Indeed, thanks to Euler's formula we usually define the principal n -th principal root of unity as

$$\omega := e^{2\pi i/n}$$

since $\frac{2\pi}{n}$ is the n -th slice of the unit circle. Furthermore, the second condition of the definition is usually not provided in terms of order of the root, and it's written as follows

$$\forall p \in [n-1] \quad \sum_{j=0}^{n-1} \omega^{jp} = 0$$

Aside from the geometric interpretation of this sum, this is a finite complex geometric series with common ratio ω^p , which implies that

- if $\omega^p = 1$, then every term is $(\omega^p)^j = 1^j = 1$ for any j , meaning that the sum is equal to

$$\sum_{j=0}^{n-1} \omega^{jp} = \sum_{j=0}^{n-1} 1 = n$$

- if $\omega^p \neq 1$, then we know that

$$\sum_{j=0}^{n-1} \omega^{jp} = \frac{1 - (\omega^p)^n}{1 - \omega^p}$$

and this ratio is equal to 0 if and only if

$$1 - (\omega^p)^n = 0 \iff \omega^{pn} = 1$$

Therefore, we have that this sum is equal to 0 if and only if $\omega^p \neq 1$ and $\omega^{pn} = 1$. However, we observe that if $\omega^p = 1$, since $p \in [n-1]$ this would imply that the order of ω is less than n , meaning that ω was not a principal root.

Now that we presented roots of unity we can finally present how the DFT matrix is usually defined.

Definition 4.3: Discrete Fourier Transform

Given a commutative ring R of dimension N , the **Discrete Fourier Transform (DFT)** matrix in R is defined as follows:

$$\forall j, k \in [0, N - 1] \quad \text{DFT}_{jk} = \omega^{-jk}$$

where ω is the principal N -th root of unity.

Therefore, in general the DFT matrix looks like this:

$$\text{DFT} := \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega^{-1} & \omega^{-2} & \dots & \omega^{-(N-1)} \\ 1 & \omega^{-2} & \omega^{-4} & \dots & \omega^{-2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{-(N-1)} & \omega^{-2(N-1)} & \dots & \omega^{-(N-1)^2} \end{pmatrix}$$

Moreover, we usually define the DFT matrix by setting $\omega = e^{\frac{2\pi i}{n}}$, thus getting

$$\forall j, k \in [0, N - 1] \quad \text{DFT}_{jk} = e^{-2\pi i j k / N}$$

Indeed, having presented the intuition behind the DFT beforehand, it's now fairly obvious the reason why the DFT matrix looks like this: its just the matrix that performs the change of basis, and since the basis of the DFT space can be defined in terms of n -th roots of unity, this is the matrix we get.

Furthermore, not surprisingly the DFT matrix is invertible, in fact we have that

$$\forall j, k \in [0, N - 1] \quad \text{IDFT}_{jk} = \text{DFT}_{jk}^{-1} = \frac{1}{N} \omega^{jk} = \frac{1}{N} e^{+2\pi i j k / N}$$

and this matrix takes the name of **Inverse Discrete Fourier Transform (IDFT)**.

Then, can't we just use the DFT matrix in quantum computations whenever we need it and be done? The problem is that the DFT matrix is clearly not unitary: if we look closely, we see that the columns of the DFT matrix are only orthogonal and not orthonormal. Thus, to solve this problem, we need to normalize the column vectors.

Definition 4.4: Quantum Fourier Transform

Given a Hilbert space \mathcal{H} of size N , the **Quantum Fourier Transform (QFT)** matrix in \mathcal{H} is defined as follows:

$$\forall j, k \in [0, N - 1] \quad \text{QFT}_{jk} = \frac{1}{\sqrt{N}} \omega^{jk}$$

where ω is the principal N -th root of unity.

We observe that the QFT matrix has positive exponents, which is just a convention employed in quantum computing. Therefore, we get the following matrix:

$$\text{QFT} := \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \cdots & \omega^{(N-1)^2} \end{pmatrix}$$

In particular, for any $|x\rangle$ basis state, the quantum Fourier transform can also be expressed as follows:

$$\text{QFT} |x\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{+2\pi i x k / N} |k\rangle$$

which directly implies that we can rewrite the QFT matrix as follows

$$\text{QFT} = \sum_{j=0}^{N-1} \left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i j k / N} |k\rangle \right) \langle j |$$

thanks to [Proposition 2.10](#).

Proposition 4.1

The QFT operator is a unitary, and in particular

$$\text{QFT}^\dagger = \sum_{j=0}^{N-1} |j\rangle \left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{-2\pi i j k / N} \langle k | \right)$$

Proof. We will leave the proof of correctness of QFT^\dagger as an exercise, and we will focus on proving that the QFT operator is indeed unitary. To prove it, is satisfies to show that

$$\text{QFT}^\dagger \text{ QFT} = \text{QFT} \text{ QFT}^\dagger = I$$

We are going to prove the leftmost product first.

$$\begin{aligned}
 \text{QFT}^\dagger \text{ QFT} &= \sum_{j=0}^{N-1} |j\rangle \left(\frac{1}{\sqrt{N}} \sum_{r=0}^{N-1} e^{-2\pi i jr/N} \langle r| \right) \sum_{k=0}^{N-1} \left(\frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} e^{2\pi i sk/N} |s\rangle \right) \langle k| \\
 &= \frac{1}{N} \sum_{j,k=0}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} e^{-2\pi i jr/N} \langle r| \right) \left(\sum_{s=0}^{N-1} e^{2\pi i sk/N} |s\rangle \right) \langle k| \\
 &= \frac{1}{N} \sum_{j,k=0}^{N-1} |j\rangle \left(\sum_{r,s=0}^{N-1} e^{2\pi i(-jr+ks)/N} \langle r|s\rangle \right) \langle k| \\
 &= \frac{1}{N} \sum_{j,k=0}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} e^{2\pi i r(k-j)/N} \right) \langle k| \quad (\langle r|s\rangle = \delta_{rs}) \\
 &= \frac{1}{N} \sum_{\substack{j,k=0: \\ j=k}}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} 1 \right) \langle k| + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} e^{2\pi i r(k-j)/N} \right) \langle k| \\
 &= \frac{1}{N} \sum_{j=0}^{N-1} |j\rangle \langle j| + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} e^{2\pi i r(k-j)/N} \right) \langle k| \\
 &= I + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} e^{2\pi i r(k-j)/N} \right) \langle k| \quad (\text{resolution of } I) \\
 &= I + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} (e^{2\pi i(k-j)/N})^r \right) \langle k| \quad (\text{resolution of } I)
 \end{aligned}$$

Now, we observe that the inner sum is a geometric series of ratio $e^{2\pi i(k-j)/N}$, and we can use its known result to simplify the calculations. However, we observe that this is true only if the ratio of the series is not equal to 1, but due to the way we split the sums we already took care of all the possible terms that could be equal to 1 so we do not need to make additional assumptions. Thus, we have that

$$\begin{aligned}
 \text{QFT}^\dagger \text{ QFT} &= I + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\sum_{r=0}^{N-1} (e^{2\pi i(k-j)/N})^r \right) \langle k| \\
 &= I + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\frac{1 - (e^{2\pi i(k-j)/N})^N}{1 - e^{2\pi i(k-j)/N}} \right) \langle k| \\
 &= I + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\frac{1 - e^{2\pi i(k-j)}}{1 - e^{2\pi i(k-j)/N}} \right) \langle k|
 \end{aligned}$$

Lastly, since $k - j$ is an integer for any $j, k \in [0, N - 1]$ — and in particular whenever $j \neq k$ — it holds that

$$e^{2\pi i(k-j)} = \cos(2\pi i(k-j)) + i \sin(2\pi i(k-j)) = 1$$

Therefore, the numerator is always equal to $1 - 1 = 0$, so the sum vanishes. Finally, we can conclude that

$$\text{QFT}^\dagger \text{ QFT} = I + \frac{1}{N} \sum_{\substack{j,k=0: \\ j \neq k}}^{N-1} |j\rangle \left(\frac{1-1}{1-e^{2\pi i(k-j)/N}} \right) \langle k| = I$$

TODO □

prove
the sec-
ond
product

4.2.1 The quantum circuit

The previous section showed how the QFT matrix operator is defined, why its unitary and its similarities with the DFT. It's finally time to address the most important question: how do we turn the QFT matrix into a quantum circuit? Assume that $N = 2^n$, and consider the definition we provided

$$\text{QFT} |x\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{+2\pi i x k / N} |k\rangle$$

The problem arises because we are using fractional exponents, however $x \in \mathbb{B}^n$. To solve this issue, we need to take a closer look at the exponent. Since $x \in \mathbb{B}^n$, there exist some bits $x_1, \dots, x_n \in \mathbb{B}$ such that x can be written as

$$x = x_1 \cdot 2^{n-1} + \dots + x_n \cdot 2^0$$

Since $k \in [0, N-1]$, we can also define such $k_1, \dots, k_n \in \mathbb{B}$, and we can see what happens when we evaluate xk/N :

$$\begin{aligned} kx/N &= \frac{(k_1 \cdot 2^{n-1} + \dots + k_n \cdot 2^0) \cdot (x_1 2^{n-1} + \dots + x_n 2^0)}{2^n} \\ &= (k_1 \cdot 2^{n-1} + \dots + k_n \cdot 2^0) \cdot \left(x_1 \cdot \frac{2^{n-1}}{2^n} + \dots + x_n \cdot \frac{2^0}{2^n} \right) \\ &= (k_1 \cdot 2^{n-1} + \dots + k_n \cdot 2^0) \cdot 0.x_1 \dots x_n \\ &= k_1 \cdot 2^{n-1} \cdot 0.x_1 \dots x_n + \dots + k_n \cdot 2^0 \cdot 0.x_1 \dots x_n \end{aligned}$$

This is true because we recall that

$$0.x_1 \dots x_n = x_1 \cdot 2^{-1} + \dots + x_n \cdot 2^{-n}$$

and since we are computing x/N and $N = 2^n$ what we get is just a “displacement of the decimal point”, but in binary. Now, we observe that

$$\forall \ell \in [n] \quad 2^{n-\ell} \cdot 0.x_1 \dots x_n = x_1 \dots x_{n-\ell}.x_{n-\ell+1} \dots x_n$$

since again, we are just moving the decimal point $n - \ell$ times to the right. Therefore, we get that

$$\begin{aligned} kx/N &= k_1 \cdot x_1 \dots x_{n-1}.x_n + \dots + k_n 0.x_1 \dots x_n \\ &= k_n \cdot 0.x_1 \dots x_n + \sum_{h=1}^{n-1} k_h \cdot x_1 \dots x_{n-h}.x_{n-h+1} \dots x_n \end{aligned}$$

we observe that we need to put $0.x_1 \dots x_n$ just because we cannot include it in the same sum. Now, let's see what happens when we put this term at the exponent:

$$\begin{aligned}
 & e^{2\pi i k x / N} \\
 &= \exp(2\pi i k x / N) \\
 &= \exp\left(2\pi i \left(k_n 0.x_1 \dots x_n + \sum_{h=1}^{n-1} k_h \cdot x_1 \dots x_{n-h} \cdot x_{n-h+1} \dots x_n\right)\right) \\
 &= \exp(2\pi i k_n 0.x_1 \dots x_n) \cdot \exp\left(2\pi i \sum_{h=1}^{n-1} k_h \cdot x_1 \dots x_{n-h} \cdot x_{n-h+1} \dots x_n\right) \\
 &= \exp(2\pi i k_n 0.x_1 \dots x_n) \cdot \exp\left(2\pi i \sum_{h=1}^{n-1} k_h \cdot (x_1 \dots x_{n-h}) + 2\pi i \sum_{h=1}^{n-1} k_h \cdot 0.x_{n-h+1} \dots x_n\right) \\
 &= \exp(2\pi i k_n 0.x_1 \dots x_n) \cdot \exp\left(2\pi i \sum_{h=1}^{n-1} k_h \cdot (x_1 \dots x_{n-h})\right) \cdot \exp\left(2\pi i \sum_{h=1}^{n-1} k_h \cdot 0.x_{n-h+1} \dots x_n\right) \\
 &= \exp(2\pi i k_n 0.x_1 \dots x_n) \cdot 1 \cdot \exp\left(2\pi i \sum_{h=1}^{n-1} k_h \cdot 0.x_{n-h+1} \dots x_n\right)
 \end{aligned}$$

The last semplifcation derives immediately from the fact that $e^{2\pi i \theta} = 1$ when θ is an integer, as we mentioned in the previous section, so that is what we are left with — since $x_1 \dots x_{n-h}$ is definitely an integer. We can proceed as follows:

$$\begin{aligned}
 & \text{QFT } |x\rangle \\
 &= \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \left(\exp(2\pi i k_n 0.x_1 \dots x_n) \cdot \exp\left(2\pi i \sum_{h=1}^{n-1} k_h \cdot 0.x_{n-h+1} \dots x_n\right) \right) |k\rangle \\
 &= \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \left(\exp(2\pi i k_n 0.x_1 \dots x_n) \cdot \exp\left(2\pi i \sum_{m=2}^n k_{n-m+1} \cdot 0.x_m \dots x_n\right) \right) |k\rangle \\
 &= \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \exp\left(2\pi i \sum_{m=1}^n k_{n-m+1} \cdot 0.x_m \dots x_n\right) |k\rangle \\
 &= \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \prod_{m=1}^n \exp(2\pi i k_{n-m+1} \cdot 0.x_m \dots x_n) |k\rangle
 \end{aligned}$$

If we look closely, this sum of products has an interesting property:

- $m = 1 \implies k_{n-m+1} = k_{n-1+1} = k_n$
- $m = n \implies k_{n-m+1} = k_{n-n+1} = k_1$

implying that it can be rewritten as follows

$$\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} (e^{2\pi i k_n \cdot 0.x_1 \dots x_n} \cdot \dots \cdot e^{2\pi i k_1 \cdot 0.x_n})$$

In other words the bits of k are *indexing* which exponentials to use in the k -th coefficient of the sum. This means that we can rewrite the last step as follows:

$$\text{QFT } |x\rangle = \frac{1}{\sqrt{N}} \bigotimes_{m=1}^n (|0\rangle + e^{2\pi i 0.x_m \dots x_n} |1\rangle)$$

Finally, the QFT written in this form can be actually implemented in a quantum circuit.

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4.3 Quantum Phase Estimation

Let's see a very useful application of the QFT introduced by Kitaev [Kit95] in 1995. By [Theorem 2.2](#) we know that the eigenvalues of a unitary operator are complex values of modulus 1. This means that any eigenvalue of a unitary operator can be written as $e^{2\pi i \varphi}$ for some real value $\varphi \in [0, 1]$ — φ being the *phase* of the complex value, i.e. the angle w.r.t. the unitary circumference.

Given a unitary operator U , and an eigenvalue $\lambda = e^{2\pi i \varphi}$, can we determine φ ? Let u be an eigenvector associated to the unknown eigenvalue λ , i.e.

$$U|u\rangle = \lambda|u\rangle = e^{2\pi i \varphi}|u\rangle$$

Now, let U^{2^k} be the quantum gate that applies the U operator 2^k times repeatedly, and define the following operator

$$\text{C-}U^{2^k} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U^{2^k}$$

This operator is the **controlled** version of U^{2^k} , and it can easily be showed by plugging $|0\rangle$ and $|1\rangle$ as first argument — alongside with some other quantum state $|\psi\rangle$

$$\begin{aligned} \text{C-}U^{2^k}(|0\rangle \otimes |\psi\rangle) &= (|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U^{2^k})(|0\rangle \otimes |\psi\rangle) \\ &= (|0\rangle\langle 0| \otimes I)|0\rangle \otimes |\psi\rangle + (|1\rangle\langle 1| \otimes U^{2^k})|0\rangle \otimes |\psi\rangle \\ &= |0\rangle \otimes |\psi\rangle \end{aligned}$$

Hence, if the first input is $|0\rangle$ the state $|\psi\rangle$ is unchanged, otherwise if the former is $|1\rangle$ we get that we actually apply U^{2^k} to $|\psi\rangle$:

$$\begin{aligned} \text{C-}U^{2^k}(|1\rangle \otimes |\psi\rangle) &= (|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U^{2^k})(|1\rangle \otimes |\psi\rangle) \\ &= (|0\rangle\langle 0| \otimes I)|1\rangle \otimes |\psi\rangle + (|1\rangle\langle 1| \otimes U^{2^k})|0\rangle \otimes |\psi\rangle \\ &= |1\rangle \otimes U^{2^k}|\psi\rangle \end{aligned}$$

Indeed, in general if we have an operator V , its controlled version can be easily built in this manner:

$$\text{C-}V = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes V$$

However, this controlled gate can also be “abused”: what happens if the control bit is a superposition of states? In particular, what happens when the control is set to

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

meaning that $|0\rangle$ and $|1\rangle$ are equally probable?

$$\begin{aligned} \text{C-}U^{2^k}(|+\rangle \otimes |\psi\rangle) &= \frac{1}{\sqrt{2}} \text{C-}U^{2^k}(|0\rangle \otimes |\psi\rangle + |1\rangle \otimes |\psi\rangle) \\ &= \frac{1}{\sqrt{2}} (\text{C-}U^{2^k}(|0\rangle \otimes |\psi\rangle) + \text{C-}U^{2^k}(|1\rangle \otimes |\psi\rangle)) \\ &= \frac{1}{\sqrt{2}} ((|0\rangle \otimes |\psi\rangle) + (|1\rangle \otimes U^{2^k}|\psi\rangle)) \end{aligned}$$

As we would expect, what happens is that the two outcomes we previously described are now equally likely, but this gets interesting if we carefully choose the target qubit. Instead of any possible $|\psi\rangle$, let's pick $|u\rangle$, the eigenvector presented at the beginning of the discussion. First, we observe that

$$U|u\rangle = e^{2\pi i\varphi}|u\rangle \implies U^{2^k}|u\rangle = (e^{2\pi i\varphi})^{2^k}|u\rangle = e^{2\pi i2^k\varphi}|u\rangle$$

Indeed, intuitively we are just performing the rotation that U performs on $|u\rangle$ exactly 2^k times. This means that

$$\begin{aligned} \text{C-}U^{2^k}(|+\rangle \otimes |u\rangle) &= \frac{1}{\sqrt{2}} ((|0\rangle \otimes |u\rangle) + (|1\rangle \otimes U^{2^k}|u\rangle)) \\ &= \frac{1}{\sqrt{2}} ((|0\rangle \otimes |u\rangle) + (|1\rangle \otimes e^{2\pi i2^k\varphi}|u\rangle)) \\ &= \frac{1}{\sqrt{2}} (|0\rangle + e^{2\pi i2^k\varphi}|1\rangle) \otimes |u\rangle \end{aligned}$$

Notice what happened here: $|0\rangle$ and $|1\rangle$ are parts of the first input, and $|u\rangle$ is the second input. In other words, by putting $|u\rangle$ as target input of the controlled gate, the target is **unchanged**, and the effect is seen on the control. We observe that this could not have been done with any other state $|\psi\rangle$ because the trick works precisely because U becomes a scalar $e^{2\pi i\varphi}$ when applied to $|u\rangle$, so it can be grouped as shown. The following quantum circuit computes the **Quantum Phase Estimation (QPE)** algorithm, and it uses precisely this trick.

Algorithm 4.1: Quantum Phase Estimation algorithm

Given a unitary operator U , and an eigenvector $|u\rangle$ of U , the algorithm returns the phase φ to which $|u\rangle$ is associated to.

```

1: function QUANTUMPHASEESTIMATION( $U, |u\rangle$ )
2:    $q_t \leftarrow |u\rangle$                                       $\triangleright q_t$  is the  $(t+1)$ -th register
3:   for  $k \in [0, t-1]$  do
4:      $q_k \leftarrow H(q_k)$ 
5:      $q_k, q_t \leftarrow U^{2^k}(q_k, q_t)$ 
6:   end for
7:    $q_0, \dots, q_{t-1} \leftarrow \text{QFT}^\dagger(q_0, \dots, q_{t-1})$ 
8:   return measure( $q_0, \dots, q_{t-1}$ )
9: end function
```

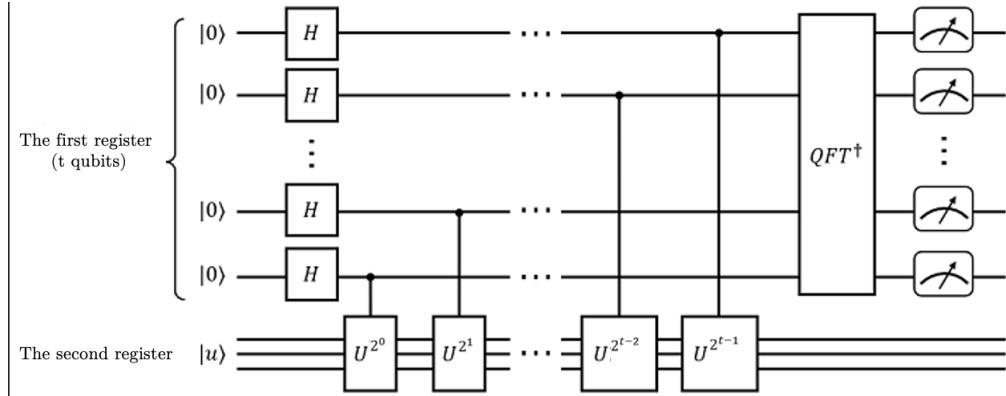


Figure 4.1: The Quantum Phase Estimation circuit.

The circuit is composed of the following elements:

- the first are $t > 0$ qubits $|0^t\rangle$ to which we apply $H^{\otimes t}$ at the beginning of the algorithm, which means now each state is set to $|+\rangle$
- the $(t+1)$ -th register is a qubit set to $|u\rangle$ — we are not going to cover the practical details about how to set a qubit to this precise quantum state
- these superpositions are used as control to the lower part of the circuit, which conditionally computes U^{2^k} for each $k \in [0, t-1]$
- at the end we compute QFT^\dagger to the first t registers

The interesting part of this circuit is that the last register remains unchanged throughout the whole computation, set precisely to $|u\rangle$, for the reason we described earlier. In fact, what happens is that what we are actually changing are the first t qubits which will be changed according to the k -th controlled gate we are using. Therefore, if we compute what happens through the QPE circuit we get the following — we will refer to the first t

registers as q_0, \dots, q_{t-1} :

$$\begin{aligned}
 & |q_0 \cdots q_{t-1}\rangle \otimes |u\rangle \\
 &= |0\rangle^{\otimes t} \otimes |u\rangle \\
 &\xrightarrow{H(q_0)} H(|0\rangle_0) \otimes |0\rangle^{\otimes t-1} \otimes |u\rangle \\
 &= |+\rangle_0 \otimes |0\rangle^{\otimes t-1} \otimes |u\rangle \\
 &= |+\rangle_0 \otimes |u\rangle \otimes |0\rangle^{\otimes t-1} \\
 &\xrightarrow{\text{C-}U^{2^0}(q_0,|u\rangle)} \text{C-}U^{2^0}(|+\rangle_0 \otimes |u\rangle) \otimes |0\rangle^{\otimes t-1} \\
 &\quad \frac{1}{\sqrt{2}}(|0\rangle_0 + e^{2\pi i 2^0 \varphi} |1\rangle_0) \otimes |u\rangle \otimes |0\rangle^{\otimes t-1} \\
 &= \frac{1}{\sqrt{2}}(|0\rangle_0 + e^{2\pi i 2^0 \varphi} |1\rangle_0) \otimes |0\rangle^{\otimes t-1} \otimes |u\rangle \\
 &= \frac{1}{\sqrt{2}}(|0\rangle_0 \otimes |0\rangle^{\otimes t-1} + e^{2\pi i 2^0 \varphi} |1\rangle_0 \otimes |0\rangle^{\otimes t-1}) \otimes |u\rangle \\
 &\xrightarrow{H(q_1)} \frac{1}{\sqrt{2}}(|0\rangle_0 \otimes H(|0\rangle_{q_1})) \otimes |0\rangle^{\otimes t-2} + e^{2\pi i 2^0 \varphi} |1\rangle_0 \otimes H(q_1) \otimes |0\rangle^{\otimes t-2}) \otimes |u\rangle \\
 &= \frac{1}{2} \left(|00\rangle_{01} + |01\rangle_{01} + e^{2\pi i 2^0 \varphi} |10\rangle_{01} + e^{2\pi i 2^0 \varphi} |11\rangle_{01} \right) \otimes |0\rangle^{\otimes t-2} \otimes |u\rangle \\
 &\xrightarrow{\text{C-}U^{2^1}(q_1,|u\rangle)} \frac{1}{2} \left(|00\rangle_{01} + e^{2\pi i 2^1 \varphi} |01\rangle_{01} + e^{2\pi i 2^0 \varphi} |10\rangle_{01} + e^{2\pi i (2^0+2^1) \varphi} |11\rangle_{01} \right) \otimes |0\rangle^{\otimes t-2} \otimes |u\rangle \\
 &\xrightarrow{\dots} \\
 &= \frac{1}{\sqrt{2^t}} \sum_{k=0}^{2^t-1} \prod_{m=1}^t e^{2\pi i k_{t-m+1} \cdot 2^{m-1} \varphi} |k\rangle \otimes |u\rangle \\
 &= \frac{1}{\sqrt{2^t}} \bigotimes_{m=1}^t \left(|0\rangle + e^{2\pi i 2^{m-1} \varphi} |1\rangle \right) \otimes |u\rangle
 \end{aligned}$$

Furthermore, we observe that $\varphi \in [0, 1)$, because as we already mentioned there is no need to consider the integral part of the phases. Thus, suppose that φ can be written through t bits $\varphi_1, \dots, \varphi_t \in \mathbb{B}$ such that

$$\varphi = 0.\varphi_1 \dots \varphi_t$$

This implies that

$$\begin{aligned}
 2^{m-1} \cdot \varphi &= 2^{m-1} \cdot 0.\varphi_1 \dots \varphi_t \\
 &= \varphi_1 \dots \varphi_{m-1} \cdot \varphi_m \dots \varphi_t
 \end{aligned}$$

Thus, since this is the exponent of $e^{2\pi i}$, we already know that

$$\exp(2\pi i \varphi_1 \dots \varphi_{m-1} \cdot \varphi_m \dots \varphi_t) = \exp(2\pi i 0.\varphi_m \dots \varphi_t)$$

therefore the tensor product can be rewritten as

$$\frac{1}{\sqrt{2^t}} \bigotimes_{m=1}^t (|0\rangle + e^{2\pi i 0.\varphi_m \dots \varphi_t} |1\rangle)$$

Very elegantly, this is exactly $\text{QFT}_t |\varphi\rangle$ we computed in the previous section (only applied in a t -dimensional space). Finally, if we place the inverse QFT — namely QFT_t^\dagger — at the end of the circuit we retrieve $|x\rangle$ itself, which is also the entire state of the system at this point (without considering $|u\rangle$). This means that if we measure each register at the end of the circuit we retrieve the bits of $\varphi_i \in \mathbb{B}^t$ — i.e. the bits that describe φ — with probability 1. In the end, we recovered the phase φ of the eigenvalue associated to $|u\rangle$ with probability 1.

As a final note, what if φ cannot be expressed in exactly t bits? It can be shown that φ can be estimated with n bits of precision through a QPE circuit composed of $n + \lceil \log(2 + \frac{1}{2\varepsilon}) \rceil$ qubits with a success probability at least $1 - \varepsilon$, for some $\varepsilon > 0$.

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4.4 Order-finding problem

The last ingredient that we need for Shor's algorithm is the **order-finding** algorithm. We recall the following property of number theory.

Proposition 4.2: Euclidean division

Given some $p \in \mathbb{N}_{>0}$, for any $n \in \mathbb{N}$ there exists unique integers $q, r \in \mathbb{Z}$ such that $0 \leq r < p$ and

$$n = p \cdot q + r$$

This is the usual division with remainder, which defines modular arithmetic, for instance

$$31 = 4 \cdot 7 + 3$$

Indeed, with equivalence classes we would write that

$$31 \equiv 3 \pmod{7}$$

Definition 4.5: Order of a number

Given a number $N \in \mathbb{N}$, for any $x \in \mathbb{Z}$ the **order** of x modulo N is the least integer r such that

$$x^r \equiv 1 \pmod{N}$$

For instance, the order of 4 modulo 7 is 3, because

$$4^3 = 64 = 9 \cdot 7 + 1 \implies 4^3 \equiv 1 \pmod{7}$$

We observe that throughout our discussion N is *not necessarily* a power of 2 as we used to assume in previous sections, however the symbol N is conventionally used in this context.

Given a number N , and a number $x < N$ that is coprime with N , can we compute its order modulo N ? This is the so called **order-finding problem**, and currently there

is no classical algorithm able to solve it in polynomial time. Let's see what quantum computation can achieve.

Consider the following unitary operator U_x that computes as follows:

$$\forall y \in \{0, 1\}^k \quad U_x |y\rangle = \begin{cases} |xy \bmod N\rangle & y < N \\ |y\rangle & y \geq N \end{cases}$$

To derive the complete operator U_x we just follow [Proposition 2.10](#):

$$\begin{aligned} U_x &= \sum_{y \in \{0,1\}^k} U_x |y\rangle \langle y| \\ &= \sum_{y < N} U_x |y\rangle \langle y| + \sum_{y \geq N} U_x |y\rangle \langle y| \\ &= \sum_{y < N} U_x |y\rangle \langle y| + \sum_{y \geq N} |y\rangle \langle y| \end{aligned}$$

We will not replace U_x inside the first sum for now in order to prove that U_x is unitary. But first, we need to present a result in number theory.

Theorem 4.1

If x and N are coprime, it holds that

$$\forall y, z \in \mathbb{Z} \quad xy \equiv xz \bmod N \iff y \equiv z \bmod N$$

Proposition 4.3

The operator U_x is unitary, and in particular

$$U_x^\dagger = \sum_{y < N} |y\rangle (U_x |y\rangle)^\dagger + \sum_{y \geq N} |y\rangle \langle y|$$

Proof. It is easy to prove the correctness of U_x^\dagger , so we are going to prove that U_x is unitary directly.

$$\begin{aligned} U_x^\dagger U_x &= \left(\sum_{y < N} |y\rangle (U_x |y\rangle)^\dagger + \sum_{y \geq N} |y\rangle \langle y| \right) \left(\sum_{z < N} U_x |z\rangle \langle z| + \sum_{z \geq N} |z\rangle \langle z| \right) \\ &= \left(\sum_{y < N} |y\rangle \langle U_x y| + \sum_{y \geq N} |y\rangle \langle y| \right) \left(\sum_{z < N} |U_x z\rangle \langle z| + \sum_{z \geq N} |z\rangle \langle z| \right) \\ &= \sum_{y, z < N} |y\rangle \langle U_x y| U_x z \rangle \langle z| + \sum_{\substack{y < N \\ z \geq N}} |y\rangle \langle U_x y| z \rangle \langle z| + \sum_{\substack{y \geq N \\ z < N}} |y\rangle \langle y| U_x z \rangle \langle z| + \sum_{y, z \geq N} |y\rangle \langle y| z \rangle \langle z| \end{aligned}$$

Now note that if $z \geq N$ and $y < N$, by definition of U_x we have that $U_x |y\rangle = |xy \bmod N\rangle$, hence it will be a basis state among $|0\rangle, \dots, |N-1\rangle$. Therefore, if $z > N$ we are guaranteed that $|z\rangle$ and $|U_x y\rangle$ are orthogonal, i.e. $\langle U_x y | z \rangle = 0$ — we recall that N is *not* the

size of the space in this context, is just a composite number, indeed the size of the space we are considering is 2^k . Therefore, we have that

$$\sum_{\substack{y < N \\ z \geq N}} |y\rangle \langle U_x y | z \rangle \langle z| = \sum_{\substack{y \geq N \\ z < N}} |y\rangle \langle y | U_x z \rangle \langle z| = 0$$

so we conclude that

$$\begin{aligned} U_x^\dagger U_x &= \sum_{y,z < N} |y\rangle \langle U_x y | U_x z \rangle \langle z| + \sum_{\substack{y < N \\ z \geq N}} |y\rangle \langle U_x y | z \rangle \langle z| + \sum_{\substack{y \geq N \\ z < N}} |y\rangle \langle y | U_x z \rangle \langle z| + \sum_{y,z \geq N} |y\rangle \langle y | z \rangle \langle z| \\ &= \sum_{y,z < N} |y\rangle \langle U_x y | U_x z \rangle \langle z| + \sum_{y,z \geq N} |y\rangle \langle y | z \rangle \langle z| \\ &= \sum_{\substack{y,z < N: \\ y \equiv z \pmod{N}}} |y\rangle \langle U_x y | U_x z \rangle \langle z| + \sum_{\substack{y,z < N: \\ y \not\equiv z \pmod{N}}} |y\rangle \langle U_x y | U_x z \rangle \langle z| + \sum_{y,z \geq N} |y\rangle \langle y | z \rangle \langle z| \end{aligned}$$

To progress, we observe that when $y, z < N$ we get that

$$\langle U_x y | U_x z \rangle = \langle xy \pmod{N} | xz \pmod{N} \rangle = \begin{cases} 1 & xy \equiv xz \pmod{N} \\ 0 & \text{otherwise} \end{cases}$$

and by [Theorem 4.1](#) we know that

$$xy \equiv xz \pmod{N} \iff y \equiv z \pmod{N}$$

thus getting

$$\begin{aligned} U_x^\dagger U_x &= \sum_{\substack{y,z < N: \\ y \equiv z \pmod{N}}} |y\rangle \langle U_x y | U_x z \rangle \langle z| + \sum_{\substack{y,z < N: \\ y \not\equiv z \pmod{N}}} |y\rangle \langle U_x y | U_x z \rangle \langle z| + \sum_{y,z \geq N} |y\rangle \langle y | z \rangle \langle z| \\ &= \sum_{\substack{y,z < N: \\ y \equiv z \pmod{N}}} |y\rangle \langle z| + \sum_{y,z \geq N} |y\rangle \langle y | z \rangle \langle z| \\ &= \sum_{\substack{y,z < N: \\ y=z}} |y\rangle \langle z| + \sum_{y,z \geq N} |y\rangle \delta_{yz} \langle z| \\ &= \sum_{y < N} |y\rangle \langle y| + \sum_{y \geq N} |y\rangle \langle y| \\ &= \sum_y |y\rangle \langle y| \\ &= I \end{aligned}$$

Now, we need to prove the opposite product



We did not provide any reason to why we defined the operator U_x as such, but before giving a geometrical intuition consider the following proposition.

Theorem 4.2

Given $N \in \mathbb{N}$, and $x \in [0, N - 1]$, if r is the order of x modulo N , it holds that

$$\forall s \in [0, r - 1] \quad |u_s\rangle = \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x^k \bmod N\rangle$$

is an eigenvector of U_x .

Proof. Fix $s \in [0, r - 1]$; to prove that $|u_s\rangle$ is an eigenvector of U_x we need to show that there exists some phase φ_s such that

$$U_x |u_s\rangle = e^{2\pi i \varphi_s} |u_s\rangle$$

because of [Theorem 2.2](#). Hence, we get that

$$\begin{aligned} U_x |u_s\rangle &= U_x \left(\frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x^k \bmod N\rangle \right) \\ &= \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} U_x |x^k \bmod N\rangle \\ &= \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x(x^k \bmod N) \bmod N\rangle \quad (x^k \bmod N < N) \\ &= \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x^{k+1} \bmod N \bmod N\rangle \\ &= \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x^{k+1} \bmod N\rangle \\ &= \frac{1}{\sqrt{r}} \cdot \frac{e^{2\pi i s/r}}{e^{2\pi i s/r}} \cdot \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x^{k+1} \bmod N\rangle \\ &= \frac{1}{\sqrt{r}} e^{2\pi i s/r} \cdot \sum_{k=0}^{r-1} e^{-2\pi i s(k+1)/r} |x^{k+1} \bmod N\rangle \\ &= \frac{1}{\sqrt{r}} \cdot e^{2\pi i s/r} \left(\sum_{k=0}^{r-2} e^{-2\pi i s(k+1)/r} |x^{k+1} \bmod N\rangle + e^{-2\pi i sr/r} |x^r \bmod N\rangle \right) \\ &= \frac{1}{\sqrt{r}} e^{2\pi i s/r} \left(\sum_{k=0}^{r-2} e^{-2\pi i s(k+1)/r} |x^{k+1} \bmod N\rangle + e^{-2\pi i s} |1\rangle \right) \quad (x^r \equiv 1 \bmod N) \\ &= \frac{1}{\sqrt{r}} e^{2\pi i s/r} \left(\sum_{m=1}^{r-1} e^{-2\pi i sm/r} |x^m \bmod N\rangle + |1\rangle \right) \\ &= \frac{1}{\sqrt{r}} e^{2\pi i s/r} \left(\sum_{m=0}^{r-1} e^{-2\pi i sm/r} |x^m \bmod N\rangle \right) \quad (|1\rangle = |x^0 \bmod N\rangle) \\ &= e^{2\pi i s/r} |u_s\rangle \end{aligned}$$

Therefore, we conclude that $\varphi_s = s/r$. □

TODO

What happens if the input of U_x is $|x^0\rangle$? By definition of our problem $x < N$, therefore

$$U_x |x^0\rangle = |x \cdot x^0 \bmod N\rangle = |x^1 \bmod N\rangle$$

Indeed in general it's easy to see that

$$U_x |x^k\rangle = |x^{k+1} \bmod N\rangle$$

In other words U_x is cycling through x 's powers, which also implies that when $k = r - 1$ we get that

$$U_x |x^{r-1}\rangle = |x^r \bmod N\rangle = |1 \bmod N\rangle$$

since r is the order of x modulo N . Moreover, as we already know these are basis states so they are both normalized and orthogonal to each other, thus the powers x form an orthonormal base of the following space

$$\mathcal{H}_r = \text{span}(|x^k \bmod N\rangle \mid k \in [0, r - 1])$$

which is a restriction of the whole Hilbert space that has exactly r dimensions. Now look again at how the eigenvectors of U_x are defined:

$$\forall s \in [0, r - 1] \quad |u_s\rangle = \frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i sk/r} |x^k \bmod N\rangle$$

This looks very similar to how we defined QFT $|x\rangle$:

$$\text{QFT } |x\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i xk/N} |k\rangle$$

Indeed, it holds that $|u_s\rangle$ is basically QFT $|s\rangle$ but taken inside \mathcal{H}_r — the only difference being the sign of the exponent, indeed it technically holds that

$$|u_s\rangle = \text{QFT}_r |-s \bmod r\rangle$$

but as we said the sign of the exponent is just a convention either sign is found in literature, we only need to be consistent with the calculations.

The most interesting part is that, as proved in the last theorem, for any fixed $s \in [0, N - 1]$ its associated phase φ_s is exactly s/r , thus if we knew how to prepare the last register of the QPE as $|u_s\rangle$ we could recover its phase, and maybe get closer to know r itself. However, we have two problems with this idea:

- there is really no easy or practical way to prepare the second register to some arbitrary state
- $|u_s\rangle$ actually depends on r itself, which actually is a very big problem on its own

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Thankfully, the following property will solve both of these issues at the same time.

Proposition 4.4

Given $N \in \mathbb{N}$, and $x \in [0, N - 1]$, if r is the order of x modulo N it holds that

$$\frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |u_s\rangle = |1\rangle$$

Proof. Through some algebraic manipulation we see that

$$\begin{aligned} \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |u_s\rangle &= \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} \left(\frac{1}{\sqrt{r}} \sum_{k=0}^{r-1} e^{-2\pi i s k / r} |x^k \bmod N\rangle \right) \\ &= \frac{1}{r} \sum_{s,k=0}^{r-1} e^{-2\pi i s k / r} |x^k \bmod N\rangle \\ &= \frac{1}{r} \sum_{s=0}^{r-1} e^{-2\pi i s \cdot 0 / r} |x^0 \bmod N\rangle + \frac{1}{r} \sum_{s=0,k=1}^{r-1} e^{-2\pi i s k / r} |x^k \bmod N\rangle \\ &= \frac{1}{r} \sum_{s=0}^{r-1} |1\rangle + \frac{1}{r} \sum_{s=0,k=1}^{r-1} e^{-2\pi i s k / r} |x^k \bmod N\rangle \\ &= \frac{1}{r} r |1\rangle + \frac{1}{r} \sum_{s=0,k=1}^{r-1} e^{-2\pi i s k / r} |x^k \bmod N\rangle \\ &= |1\rangle + \frac{1}{r} \sum_{k=1}^{r-1} |x^k \bmod N\rangle \sum_{s=0}^{r-1} e^{-2\pi i s k / r} \\ &= |1\rangle + \frac{1}{r} \sum_{k=1}^{r-1} |x^k \bmod N\rangle \sum_{s=0}^{r-1} (e^{-2\pi i k / r})^s \end{aligned}$$

As we did for the proof of [Proposition 4.1](#), because of how we split the sums we know that $k \neq 0$ hence $e^{-2\pi i k / r} \neq 1$ because k/r is not an integer (since $k \in [1, r - 1]$), therefore we get that

$$\begin{aligned} \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |u_s\rangle &= |1\rangle + \frac{1}{r} \sum_{k=1}^{r-1} |x^k \bmod N\rangle \frac{1 - (e^{-2\pi i k / r})^r}{1 - e^{-2\pi i k / r}} \\ &= |1\rangle + \frac{1}{r} \sum_{k=1}^{r-1} |x^k \bmod N\rangle \frac{1 - e^{-2\pi i k}}{1 - e^{-2\pi i k / r}} \\ &= |1\rangle + \frac{1}{r} \sum_{k=1}^{r-1} |x^k \bmod N\rangle \frac{1 - 1}{1 - e^{-2\pi i k / r}} \\ &= |1\rangle \end{aligned}$$

□

Indeed, this property is incredibly useful because we can provide $|1\rangle$ to the lower register of the QPE circuit instead of a single eigenvector, in order to compute the same algorithm but to all the eigenvectors **simultaneously**. We observe that $|1\rangle$ is essentially a superposition of all the eigenvectors of U_x , which means that when fed to C- $U_x^{2^k}$ as target qubit we don't really get $|1\rangle$ back, indeed

$$\begin{aligned}
 \text{C-}U_x^{2^k}(|+\rangle_0 \otimes |1\rangle_1) &= \frac{1}{\sqrt{2}} \left(|0\rangle_0 \otimes |1\rangle_1 + |1\rangle_0 \otimes U_x^{2^k} |1\rangle_1 \right) \\
 &= \frac{1}{\sqrt{2}} \left(|0\rangle_0 \otimes |1\rangle_1 + |1\rangle_0 \otimes U_x^{2^k} \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |u_s\rangle_1 \right) \\
 &= \frac{1}{\sqrt{2}} \left(|0\rangle_0 \otimes |1\rangle_1 + |1\rangle_0 \otimes \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} U_x^{2^k} |u_s\rangle_1 \right) \\
 &= \frac{1}{\sqrt{2}} \left(|0\rangle_0 \otimes |1\rangle_1 + |1\rangle_0 \otimes \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} e^{2\pi i 2^k s / r} |u_s\rangle_1 \right) \\
 &= \frac{1}{\sqrt{2}} \left(|0\rangle_0 \otimes \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |u_s\rangle_1 + |1\rangle_0 \otimes \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} e^{2\pi i 2^k s / r} |u_s\rangle_1 \right) \\
 &= \frac{1}{\sqrt{2r}} \sum_{s=0}^{r-1} \left(|0\rangle_0 + e^{2\pi i 2^k s / r} |1\rangle_0 \right) \otimes |u_s\rangle_1
 \end{aligned}$$

Nevertheless, notice what happened here: we entangled the control qubit with the target qubit, such that now the target *picked up the phase* $e^{2\pi i 2^k s / r}$ — exactly as the standard QPE — and we are still preserving the superposition of eigenvectors $|u_s\rangle$. This is exactly what we need, however it also means that the result at the end of the circuit is not very straightforward: in standard QPE the resulting state is just the tensor product of the single control qubits because they are independent from each other, but here we are entangling all the control and the target qubits together at each application of C- $U_x^{2^k}$. Hence, we need to compute what happens step by step:

fallo

TODO

$$\begin{aligned}
 &= \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} \frac{1}{\sqrt{2^t}} \bigotimes_{m=1}^t \left(|0\rangle + e^{2\pi i 2^{m-1} s / r} |1\rangle \right) \otimes |u_s\rangle \\
 &= \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} \frac{1}{\sqrt{2^t}} \bigotimes_{m=1}^t \left(|0\rangle + e^{2\pi i 0 \cdot \varphi_{sm} \dots \varphi_{st}} |1\rangle \right) \otimes |u_s\rangle \\
 &= \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} \text{QFT}_t |\varphi_s\rangle_{q_0 \dots q_{t-1}} \otimes |u_s\rangle \\
 &\xrightarrow{\text{QFT}_t^\dagger(|q_0 \dots q_{t-1}\rangle)} \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |\varphi_s\rangle \otimes |u_s\rangle
 \end{aligned}$$

assuming that $\varphi_s = s/r$ can be written through t bits. This entangled quantum state is exactly what we want, because now by measuring the first t registers we get that for each $s \in [0, r-1]$ they will collapse into $|\varphi_s\rangle$ with probability $\frac{1}{r}$, and the last register will

collapse into $|u_s\rangle$ which is exactly the eigenvector associated to $e^{2\pi i \varphi_s}$. This proves that we truly computed the phases of all the possible eigenvectors simultaneously.

We are almost done. We now know that we can retrieve $\varphi_s = s/r$ for each $s \in [0, r - 1]$ without even knowing a single eigenvector of U_x , but there is a problem. Say that we want to find the order of $x = 3$ modulo $N = 11$, which is $r = 5$, and suppose that the true phase that the algorithm *should* output is

$$\varphi_s = \frac{s}{r} \implies \varphi_2 = \frac{2}{5} = 0.4$$

The QPE algorithm, however, cannot output this exact value, because 0.4 cannot be written precisely in binary — in particular, the reason is that 5 does not divide 2^t for any t . This means that our algorithm will return an *approximation* of φ_2 . Say that we are working with 6 registers of precision and fix $t = 6$; then QPE will output the closest approximation of 0.4 with 6 bits:

$$\tilde{\varphi}_2 = 0.40625 = \frac{13}{32}$$

Now, it would be a mistake to assume that $r = 32$! How do we proceed?

Definition 4.6: Continued fraction

Given a rational number $x \in \mathbb{Q}$, the continued fraction of x is composed by a set of numbers $a_0, \dots, a_n \in \mathbb{N}$ — where $a_n \neq 0$ — such that

$$x = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\ddots + \cfrac{1}{a_n}}}}$$

The continued fraction is usually denoted with the following notation

$$x = [a_0; a_1, a_2, \dots, a_n]$$

Moreover, each “partial” continued fraction

$$\begin{aligned} &[a_0] \\ &[a_0; a_1] \\ &[a_0; a_1, a_2] \\ &\dots \\ &[a_0; a_1, a_2, \dots, a_n] \end{aligned}$$

is called **convergent** of the original number.

For instance, the number $\frac{338}{121}$ can be written as follows:

$$\frac{338}{121} = [2; 1, 3, 1, 5, 4]$$

and its convergents are

$$\begin{aligned} [2] \\ [2; 1] \\ [2; 1, 3] \\ \dots \\ [2; 1, 3, \dots, 4] \end{aligned}$$

We will use continued fractions to recover r from $\tilde{\varphi}_s$. Suppose that QPE outputs $\tilde{\varphi}_2 = \frac{13}{32}$ as in the previous example. Without going into the details, there is a classical algorithm which is able to recover its continued fraction in $O(L^3)$ time — where $L = \lceil \log N \rceil$. Thus, we get that

$$\tilde{\varphi}_2 = 0 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{6}}} = [0; 2, 2, 6]$$

Now, to recover $\frac{2}{5}$ we just need to compute the convergents:

$$\begin{aligned} [0] &= 0 \\ [0; 2] &= \frac{1}{2} \\ [0; 2, 2] &= \frac{2}{5} \\ [0; 2, 2, 6] &= \frac{13}{32} \end{aligned}$$

Finally, since we know that r is the order of x modulo N , we just need to pick the convergent with the smallest denominator r such that $x^r \equiv 1 \pmod{N}$. In our example we had $x = 3$ and $N = 11$, thus

$$\begin{aligned} 3^2 &\equiv 9 \not\equiv 1 \pmod{11} \\ 3^5 &\equiv 243 \equiv 1 \pmod{11} \end{aligned}$$

This is how we can recover $r = 5$ — to be precise, there are theoretical results which guarantee that $\frac{2}{5}$ shows among the convergents of $\frac{13}{32}$ but this is outside the scope of our discussion.

4.5 Shor's algorithm

TODO

intro

Theorem 4.3: Fundamental Theorem of Arithmetic

Given any $N \in \mathbb{N}$, there exists unique $p_1, \dots, p_m \in \mathbb{P}$ primes and $\alpha_1, \dots, \alpha_m$ exponents — for some $m \in \mathbb{N}$ — such that

$$N = p_1^{\alpha_1} \cdot \dots \cdot p_m^{\alpha_m}$$

The set of primes $p_1, \dots, p_m \in \mathbb{P}$ is called **prime factorization** of N . The **Integer Factorization Problem (IFP)** asks to retrieve the prime factorization of any given $N \in \mathbb{N}$.

Theorem 4.4

Given any L -bit long composite natural number $N \in \mathbb{N}$, let $x \in [2, N]$ different from $N - 1$ be a solution to the equation

$$x^2 \equiv 1 \pmod{N}$$

Then, at least one of $\gcd(x - 1, N)$ and $\gcd(x + 1, N)$ is a non-trivial factor of N that can be computed using $O(L^3)$ operations.

Theorem 4.5

Given any $N \in \mathbb{N}$ odd composite positive integer with m prime factors, let $x \in_R [1, N - 1]$ such that $\gcd(1, N - 1) = 1$. Then, if r is the order of x modulo N , it holds that

$$\Pr[r \text{ is even and } x^{r/2} \not\equiv 1 \pmod{N}] \geq 1 - \frac{1}{2^m}$$

TODO

TODO

TODO

write the alg and explain stuff?

size of QPE

write QPE alg

size of Ux gates

4.6 Furhter considerations on Grover's algorithm

At the end of the previous chapter we ended our discussion of Grover's algorithm by noticing how the G operator was actually performing a *rotation* of an angle 2θ , but there is still something left to be explained. Shor developed his algorithm in 1994, while Grover presented his own in 1996, however in the same year he stated the following famous sentence

It might be possible to combine the search scheme of this paper with Shor [Sho] and other quantum mechanical algorithms to design faster algorithms

which subsequently lead many to believe that he actually took inspiration for his algorithm.

Let's try to understand how we can actually employ some of the ideas used in Shor's algorithm for Grover's quantum search. Recall that in [Proposition 3.3](#) we proved that the Grover operator can be rewritten as follows:

$$G = \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix}$$

We observe the following property.

Proposition 4.5

The eigenvalues of G are $e^{\pm 2\theta i}$.

Proof. The characteristic polynomial of G is given by

$$\begin{aligned} p(\lambda) &= \det(G - \lambda I) \\ &= \det \left(\begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \right) \\ &= \det \begin{pmatrix} \cos 2\theta - \lambda & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta - \lambda \end{pmatrix} \\ &= \lambda^2 - 2\lambda \cos 2\theta + \cos^2 2\theta + \sin^2 2\theta \\ &= \lambda^2 - 2\lambda \cos 2\theta + 1 \end{aligned}$$

and solving for $p(\lambda) = 0$ yields the following two eigenvalues:

$$\begin{aligned} \lambda &= \frac{2 \cos 2\theta \pm \sqrt{4 \cos^2 2\theta - 4}}{2} \\ &= \cos 2\theta \pm \sqrt{\cos^2 2\theta - 1} \\ &= \cos 2\theta \pm \sqrt{-\sin^2 2\theta} \\ &= \cos 2\theta \pm i \sin 2\theta \\ &= e^{\pm 2\theta i} \end{aligned}$$

□

This means that we can use the QPE algorithm with the matrix G in order to obtain an estimate of θ ! In particular, with this information we can actually solve two problems at once:

- we can determine an estimate how many iterations of Grover's algorithm we need to run, since

$$k = \frac{\pi}{4\theta} - \frac{1}{2}$$

- we can also evaluate an estimate on M , the number of solutions, since

$$\theta = \arcsin \sqrt{\frac{M}{N}} \iff M = N \sin^2 \theta$$

The problem of estimating M is usually referred to as **quantum counting** in the literature, since the output is the number of solutions inside the given array.

TODO

drawing

It can be proven that the quantum counting circuit estimates $\pm 2\theta$ — to be precise, it actually estimates 2θ or $2\pi - 2\theta$ since QPE does not return negative angles — to a degree of accuracy up to a desired 2^{-m} with probability at least $1 - \varepsilon$. Moreover, it can be shown that

$$|\tilde{M} - M| < \left(2\sqrt{MN} + \frac{N}{2^{m+1}} \right) 2^{-m}$$

where \tilde{M} is the estimated value of M through the QPE algorithm. For instance, choosing $m = \lceil \frac{n}{2} \rceil + 1$ and $\varepsilon = \frac{1}{6}$, we get that $t = \lceil \frac{n}{2} \rceil + 3$ and an estimation of M with an error of about

$$|\tilde{M} - M| < \sqrt{\frac{M}{2}} + \frac{1}{4} = O(\sqrt{M})$$

with only $O(2^t) = O(\sqrt{N})$ iterations of the Grover operator, i.e. array accesses. Classically, to know the value of M with the same error in the estimate we would necessarily need $O(N)$ accesses.

Lastly, another problem that quantum counting solves is knowing if M is 0 or not. Indeed, Grover's algorithm relies on the assumption that $M \neq 0$, i.e. there are solution elements, otherwise the procedure actually does nothing.

4.7 Variational Quantum Algorithms

While algorithms like Grover and Shor's show the theoretical power of quantum computing, it must be pointed out that they assume access to **large** and **error-free** quantum machines, hardware that *does not yet exist*. In fact, today's quantum devices are known as **Noisy Intermediate-Scale Quantum (NISQ)** machines, which have a limited number of qubits, noisy gates, short coherence times, and can only run shallow circuits before errors overwhelm the computation. In this section we will present a fairly recent approach that allows to work with such noisy machines, called **Variational Quantum Algorithms (VQAs)**. They are a type of quantum algorithms that are designed to work on NISQ devices we have today. By combining short, parameterized quantum circuits with classical optimization, VQAs allow the quantum computer to handle tasks it performs best — such as exploring complex quantum states and measuring key properties — assisted by a classical computer that iteratively adjusts the circuit parameters. This hybrid method tolerates noise and imperfections, making it possible to obtain useful results even with limited, error-prone hardware.

VQAs are a leading method for achieving quantum advantage on today's NISQ devices. They work by combining shallow, parameterized quantum circuits — well-suited to noisy hardware — with classical optimization techniques that adjust those parameters. This hybrid quantum-classical strategy resembles **machine-learning** approaches like neural networks and helps manage NISQ constraints while avoiding the deep circuits required by fully fault-tolerant quantum algorithms.

VQAs have been explored for a wide range of quantum computing applications and may offer the best chance for near-term quantum advantage. Due to the inherent versatility of VQAs, there is a wide variety of different algorithmic structures with different levels of complexity. Nevertheless, most of VQAs share the same basic elements. A VQA begins

with a clearly defined task and, if needed, relevant training data. The first step is to design a **cost function** C that captures what it means to solve the problem.

Next, it must be chosen an **ansatz**, a German term that can be translated to *approach* or *attempt*. In the context of physics and mathematics, an ansatz is kind of an initial estimate to the solution of the problem considered. For instance, given a set of experimental data that looks to be clustered about a line, a *linear ansatz* could be made to find the parameters of the line by a *least squares* curve fit. In other words, if experimental data looks linear, we might choose a linear model

$$y = mx + b$$

because we believe that the solution lives somewhere in the “space of all straight lines”. Thus, in the quantum context specifically, the ansatz is the **family of quantum states** we allow the VQA to explore

$$|\psi(\theta)\rangle = U(\theta) |\psi_0\rangle$$

for some initial state $|\psi_0\rangle$, and a set of parameters θ of the model — θ is not an angle here! This means that choosing the structure of the circuit *is* the ansatz itself. In fact, this is the reason why choosing an appropriate ansatz is one of the most important steps of the whole process, and there are a wide range of ansatze that are currently being studied in order to model different type of problems. Cerezo, Arrasmith, Babbush, et al. [CAB+20] compiled a detailed list of the best known ansatze depending on the application of the VQA.

The algorithm then trains these parameters through a hybrid quantum-classical optimization loop, seeking the values

$$\theta^* = \arg \min_{\theta} C(\theta)$$

that minimize the cost function chosen. The quantum computer then evaluates the cost, and a classical optimizer updates the parameters according to a preferred optimization strategy — classical **Stochastic Gradient Descent (SGD)** is usually employed but newer alternatives are being developed in recent years that are “gradient-free”.

VQAs are highly flexible because they support task-oriented programming, making them suitable for nearly every major application envisioned for quantum computers. In fact, they are powerful enough to enable **universal quantum computation**. A quantum model is said to be **universal** if it can approximate any unitary operation on any number of qubits to arbitrary accuracy, only using some kind of restricted architecture. In some sense, it is the quantum analog of what being a *universal gate* means with classical gates.

4.7.1 Variable Quantum Eigensolver

The best-known application of VQAs is by far the so called **Variable Quantum Eigensolver (VQE)** since it was the very first proposed VQA, developed to provide a near-term application for VQAs.

First, let’s describe the problem we are interested in solving. In chemistry and many other fields, we are often interested in finding the fundamental physical properties of the

system we are considering. Interestingly, such properties can be directly evaluated from the eigenvalues of the **Hamiltonian**, which is an operator that we briefly introduced in [Postulate 2.3](#). The Hamiltonian of a system represents its total energy — including kinetic energy, potential energy and the interactions between particles. This fact derives from the **time-independent Schrödinger equation (TISE)**:

$$H |\psi\rangle = E |\psi\rangle$$

which is used when looking at stationary states — states whose probability distributions don't change over time. In this formula, we have that

- H is the Hamiltonian
- E is an eigenvalue of H , which is the energy of $|\psi\rangle$
- $|\psi\rangle$ is an eigenvector associated to E , which is the stationary state we are considering

Each eigenvalue E of H tells us an allowed energy level of the system, and we are interested in the *lowest one*, which is called **ground-state energy**, often denoted as E_G . While higher eigenvalues describe **excited states** that govern how molecules absorb and emit light, E_G describes a molecule's stability, preferred structure and how it participates in chemical reactions. This is the eigenvalue we are interested in, and it will be the main focus of our discussion. Determining the ground-state energy is essential for understanding spectroscopy, photochemistry, and materials used in solar cells or sensors. Moreover, beyond chemistry many problems in physics, materials science, and engineering reduce to eigenvalue calculations as well, such as the behavior of electrons in solids and the vibrations of mechanical structures.

What is the problem in finding the eigenvalues of H then? We observe that when we have a system of n particles we require a Hilbert space of dimension 2^n , which means that the size of the Hamiltonian is $2^n \times 2^n$. This exponential growth makes the search for eigenvalues **classically intractable**. Traditional approximate methods help but cannot achieve efficient, exact solutions for large systems. Luckily, quantum computing offers a promising path forward.

Actually, we already know a quantum algorithm that is able to yield the eigenvalue of a unitary operator: it's the QPE. Indeed, this algorithm *does* provide exponential speedups w.r.t. classical approaches, however it requires long coherent evolution and *extremely deep circuits*, making it impractical for near-term devices. Today, in the NISQ era, QPE is still not practical. However, in 2014 Peruzzo, McClean, Shadbolt, et al. [[PMS+14](#)] published a landmark paper, which proposed a VQA that avoids the long coherent runtimes required by QPE.

From a theoretical point of view, the idea is fairly straightforward: we want to find the state $|\psi^*\rangle$ that minimizes the eigenvalue, in order to find E_G . But first, let's consider a more general scenario: let A be any observable (i.e. a self-adjoint operator), and consider its expected value $\langle A \rangle$. In [Proposition 2.14](#) we already proved that if the current state is $|\psi\rangle$ it holds that

$$\langle A \rangle = \langle \psi | A \psi \rangle$$

We are interested in finding the state $|\psi^*\rangle$ that will yield the lowest possible eigenvalue of A after measuring the latter. We observe that

$$\begin{aligned}\langle\psi|A\psi\rangle &= \langle A \rangle \\ &= \mathbb{E}[A \mid |\psi\rangle] \\ &= \sum_{i=1}^m \lambda_i \Pr[A = \lambda_i \mid |\psi\rangle] \\ &\geq \min_{i \in [m]} \lambda_i \\ &= \lambda_{\min}\end{aligned}$$

with the equality holding if $|\psi\rangle = |\psi^*\rangle$. This means that by searching for

$$|\psi^*\rangle = \arg \min_{|\psi\rangle \in \mathcal{H}} \langle\psi|A\psi\rangle$$

we can immediately find λ_{\min} . It is easy to see that this idea is clearly applicable for finding E_G since H is self-adjoint, thus

$$|\psi^*\rangle = \arg \min_{|\psi\rangle \in \mathcal{H}} \langle\psi|H\psi\rangle \implies H|\psi^*\rangle = E_G|\psi^*\rangle$$

where E_G is the lowest eigenvalue of H , by definition. As a consequence, the idea of the VQE is to set the cost function as

$$C(\theta) = \langle\psi(\theta)|H\psi(\theta)\rangle$$

where in this case $|\psi(\theta)\rangle$ is the “trial” state that has to be defined as

$$|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$$

where $U(\theta)$ represents the ansatz of choice. Therefore, we are interested in finding the best parameters such that

$$\theta^* = \arg \min_{\theta} \langle\psi(\theta)|H\psi(\theta)\rangle$$

We observe that there is no universal ansatz for the VQE, as there are multiple variants that have been developed depending on the specific Hamiltonian of interest — different Hamiltonians may have different structures, entanglement patterns and symmetries. In conclusion, from a theoretical standpoint of view the VQE aims at minimizing $C(\theta)$ by computing the cost with a NISQ machine, and by optimizing θ through a classical computer.

In particular, we observe that the evaluation of the cost depends on the value of $\langle H \rangle$, and the best way we have to evaluate this quantity is by repeatedly measuring H . However, due to the size of H and the noise of the machines this step is often implemented with a better alternative. In fact, there is a very useful property of Hamiltonians that we can leverage: any Hamiltonian can be written as linear combination of products of Pauli matrices

$$H = \sum_j h_j \prod_k \sigma_{\alpha,jk}$$

where $\alpha \in \{x, y, z\}$. The original approach of the VQE only considers Hamiltonians that can be written as a sum of a polynomial number of terms. This property has two practical implications:

- first, the product of two Pauli matrices is a Pauli matrix multiplied by some phase, as the table below shows

	I	X	Y	Z
I	I	X	Y	Z
X	X	I	iZ	$-iY$
Y	Y	$-iZ$	I	iX
Z	Z	iY	$-iX$	I

which means that we can rewrite the sum as follows

$$H = \sum_k h'_k \sigma_{\alpha,k}$$

for some new coefficients h'_k

- second, by linearity of expectations it holds that

$$\langle H \rangle = \sum_{k=1} h'_k \langle \sigma_{\alpha,k} \rangle$$

which means that in order to compute the cost $C(\theta)$ we can instead evaluate the following

$$C(\theta) = \langle H \rangle = \langle \psi(\theta) | H \psi(\theta) \rangle = \sum_{k=1} c_k \langle \psi(\theta) | \sigma_{\alpha,k} \psi(\theta) \rangle$$

This is much more feasible on current NISQ hardware, as measuring each $\langle \sigma_{\alpha,k} \rangle$ only requires shallow circuits. We observe that this is an oversimplification and we are glossing over a lot of details, both from a theoretical and physical point of view, but such specifics are definitely outside the scope of this discussion as they would require an entire chapter on their own.

The last thing that we are going to mention about the VQE is its versatility. We showed how with this technique we are able to determine the ground-state energy of a Hamiltonian H , which is useful to know in various scientific research areas. However, in reality we observe that the method we outlined *does not depend* on the meaning of H . In fact, H really can be any self-adjoint operator that can be written as sum of “easier” operators to measure. Consider any cost function $S(x)$ that we seek to minimize; what we need is a matrix H_S whose eigenvalues are exactly the possible values that $S(x)$ can assume. Hence, by using the same trick that we used in the [Born rule](#) it suffices to consider a matrix whose [Spectral decomposition](#) is exactly

$$H_S = \sum_{y \in Y} S(y) |y\rangle \langle y|$$

Thus, by construction this immediately implies that

$$H_S |y\rangle = S(y) |y\rangle$$

Therefore, by executing the VQE on H_S we are actually finding the lowest value of $S(y)$:

$$\begin{aligned}\langle \psi | H_S \psi \rangle &= \langle H_S \rangle \\ &= \mathbb{E} H_S \mid |\psi\rangle \\ &= \sum_{y \in Y} S(y) \Pr[H_S = S(y) \mid |\psi\rangle] \\ &\geq \min_{y \in Y} S(y)\end{aligned}$$

In the end, we can simply run the VQE algorithm with

$$C(\theta) = \langle H_S \rangle = \langle \psi(\theta) | H_S \psi(\theta) \rangle$$

to get an approximation of the minimum value for our original cost function. This strategy is used to approximate various classically intractable computational problems outside chemistry and physics, such as

- **max-cut** problems, in which H_S encodes the cut costs
- **combinatorial optimization** problems, in which H_S encodes the constraints

The following procedure is a high-level overview of the implementation of this idea.

Algorithm 4.2: Optimization through VQE

Given a cost function S , and a fixed parameter N , the algorithm returns an approximation of $\min_{y \in Y} S(y)$.

```

1: function VQEOPTIMIZATION( $S, N$ )
2:    $\theta \leftarrow \theta_0$ 
3:   while true do
4:     Generate circuit  $Q_\theta$  from ansatz based on  $\theta$ 
5:      $c_\theta \leftarrow []$ 
6:     for  $i \in [N]$  do
7:        $|\psi(\theta)\rangle \leftarrow Q_\theta |0^n\rangle$ 
8:        $c_i \leftarrow H_C$  measured on  $|\psi(\theta)\rangle$ 
9:        $c_\theta.append(c_i)$ 
10:    end for
11:     $\hat{c}_\theta \leftarrow \text{avg}(c_\theta)$ 
12:    if classical machine determines that  $\hat{c}_\theta$  is ok then
13:      return  $\theta$ 
14:    end if
15:     $\theta \leftarrow \theta'$                                  $\triangleright \theta'$  computed classically
16:  end while
17: end function
```

5

Quantum Information Science

TODO

write introduction

5.1 Quantum Key Distribution

Why is Shor's algorithm so important? Most widely used **public-key cryptography** algorithms rely on the difficulty of one of the three following mathematical problems:

- the Integer Factorization problem
- the Discrete Logarithm problem
- the Elliptic-Curve Discrete Logarithm problem

In particular, all of the problems are currently *very hard* to solve efficiently, and basically any modern cryptosystem is based on the fact that we don't know any fast-enough algorithm that is able to solve them. However, all of these could be easily solved on a sufficiently powerful quantum computer that runs Shor's algorithm, as we already seen.

explain details

Nevertheless, at the time of writing quantum computers lack the processing power to break widely used cryptographic algorithm, so we are still safe from a world without crypto. However, because of the length of time required for migration to **quantum-safe cryptography**, are already designing new algorithms to prepare for the so called **Q-Day**, the day when current algorithms will be vulnerable to quantum computing attacks. For example, NIST already initiated a process to solicit, evaluate and standardize one or more quantum-resistant public-key cryptography algorithms".

In this chapter we will cover

is a **Quantum Key Distribution (QKD)** protocol. In particular, we are interested in finding secure protocols that allow two parties to share a *private key* quantum-safely.

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5.1.1 The No-cloning theorem

Before explaining any protocol however, we need to talk about a theorem that we did not properly discuss in [Section 1.3.2](#), namely the **No-cloning theorem**. In particular, we stated that there is no quantum transformation that copies any quantum state. Now that we have the mathematical tools to prove the theorem, we can actually show the real formulation of the theorem. But first, let's try to understand what it means to “clone” a qubit. Say that we have a qubit set to some unknown superposition of states $|\chi\rangle$ that we would like to clone; in other words, we need an ancilla qubit $|\gamma\rangle$ and some operator U (which must be unitary) such that

$$U(|\chi\rangle \otimes |\gamma\rangle) = |\chi\rangle \otimes |\chi\rangle$$

Essentially, the ancilla qubit is used to store the clone of $|\chi\rangle$. We observe that the initial state of the ancilla can be considered to be some fixed superposition, since the qubit $|\chi\rangle$ is *unknown* and we want U to work on any possible state. However, the No-cloning theorem states that such a transformation U cannot exist if the choice of the possible state for $|\chi\rangle$ isn't restricted enough.

Theorem 5.1: No-cloning theorem

Let \mathcal{H} be a Hilbert space, and let $S \subseteq \mathcal{H}$ be a set of vectors. If S contains two distinct non-orthogonal vectors, there is no unitary operator

$$U : \mathcal{H} \otimes \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}$$

such that there exists a fixed vector $|\gamma\rangle \in \mathcal{H}$ such that

$$\forall |\chi\rangle \in S \quad U(|\chi\rangle \otimes |\gamma\rangle) = |\chi\rangle \otimes |\chi\rangle$$

Proof. By way of contradiction, suppose that there exists a unitary transformation U for which there exists a fixed $|\gamma\rangle \in \mathcal{H}$ that can be universally used as ancilla qubit to copy any $|\chi\rangle \in S$. Moreover, let $|\psi\rangle, |\phi\rangle \in S$ two distinct vectors such that $\langle\psi|\phi\rangle \neq 0$ meaning that they are non-orthogonal. Because U is unitary, by [Proposition 2.8](#) we know that it must preserve the scalar product, meaning that

$$\forall x, y \in \mathcal{H} \quad \langle Ux | Uy \rangle = \langle x | y \rangle$$

In particular, this must hold for

$$\begin{aligned} x &= |\psi\rangle \otimes |\gamma\rangle \\ y &= |\phi\rangle \otimes |\gamma\rangle \end{aligned}$$

however we see that

$$\begin{aligned} &\langle U(|\psi\rangle \otimes |\gamma\rangle) | U(|\phi\rangle \otimes |\gamma\rangle) \rangle = \langle \psi \otimes \gamma | \phi \otimes \gamma \rangle \\ \iff &\langle \psi \otimes \psi | \phi \otimes \phi \rangle = \langle \psi \otimes \gamma | \phi \otimes \gamma \rangle \\ \iff &\langle \psi | \phi \rangle \langle \psi | \phi \rangle = \langle \psi | \phi \rangle \langle \gamma | \gamma \rangle \\ \iff &\langle \psi | \phi \rangle = 1 \quad (\langle \phi | \psi \rangle \neq 0) \\ \iff &|\psi\rangle = |\phi\rangle \end{aligned}$$

This means that $|\psi\rangle$ and $|\phi\rangle$ are actually the same vector, contradicting the fact that we chose them distinct in S . \square

The most important details of this formulation are the following:

- we require S to have at least two distinct non-orthogonal vectors
- the theorem is defined on a *set* of vectors S which may not necessarily be the whole Hilbert space considered

The second observation is crucial because depending on the choice of S “cloning” is *possible*. Indeed, suppose that we restrict our interest in the set of the only two states $|0\rangle$ and $|1\rangle$, i.e. $S = \{|0\rangle, |1\rangle\}$. In this scenario, we *can* actually define an operator such that

$$\exists |\gamma\rangle \quad \forall |\chi\rangle \in \{|0\rangle, |1\rangle\} \quad U(|\chi\rangle \otimes |\gamma\rangle) = |\chi\rangle \otimes |\chi\rangle$$

and it’s just a CNOT with $y = |0\rangle$:

$$\text{CNOT}(|0\rangle \otimes |0\rangle) = |0\rangle \otimes |0\rangle$$

$$\text{CNOT}(|1\rangle \otimes |1\rangle) = |1\rangle \otimes |1\rangle$$

This operation is called **duplication**, and depending on the set S it can be performed without any issue. As a final note, we observe that the No-cloning theorem is usually stated as follows.

Corollary 5.1

There is no quantum transformation that copies an unknown quantum state.

This is just the particular case in which $S = \mathcal{H}$, and \mathcal{H} obviously contains non-orthogonal pair of distinct states.

The hypothesis of the No-cloning theorem regarding the choice of S is used strategically by the BB84 protocol, as we will see in the next section.

5.1.2 Measurements

Before describing the next step of the protocol, we need to do a step back and talk about *measurement* in greater detail. Each time we discussed “measuring” we never actually mentioned that when we are *physically* performing a measurement what we are really doing is applying a “polarizing lens” to the final state. For instance, this operation can be implemented through **Faraday rotators**, which leverage the **Faraday effect**:

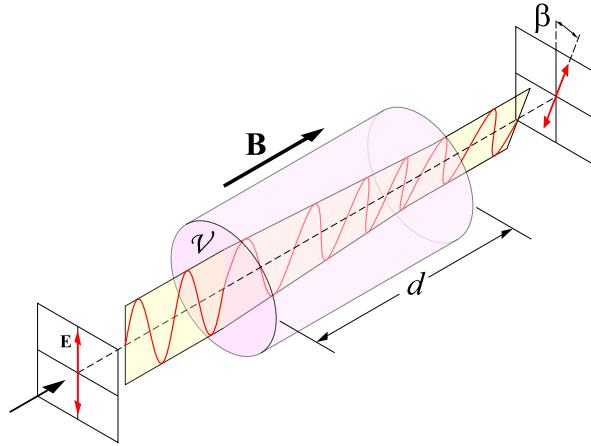


Figure 5.1: A Faraday polarization rotator.

This is important because it means that when we talk about measurement we need to define the “angle” at which we perform it. Mathematically speaking, this is equivalent to defining the **basis of choice** for the measurement — we always consider orthonormal bases only, so all the possible bases of a space are identical up to a rotation. Indeed, the importance of the choice of the basis can be illustrated through the BB84 protocol itself.

- If we have a qubit in the state $|\phi\rangle = |+\rangle$, we know that the probability of getting either $|0\rangle$ or $|1\rangle$ when measured in the Z basis is precisely 50% for both outcomes because

$$\Pr[\text{measure}(|\phi\rangle = |0\rangle)] = |\langle 0|+\rangle|^2 = \frac{1}{2}$$

- Now, consider the orthonormal basis formed by the vector $|+\rangle$ and $|-\rangle$ — which is usually called **X basis**; we observe that this space is just a rotation of 45° clockwise of the Z basis. This space is interesting: when we measure a qubit $|\phi\rangle$ set to the state $|0\rangle$ in the Z basis we get $|0\rangle$ with 100% certainty, but in this space we have that

$$\begin{aligned} \Pr[\text{measure}(|\phi\rangle = |+\rangle)] &= |\langle 0|+\rangle|^2 \\ &= \left| \frac{1}{\sqrt{2}} \langle 0| (|0\rangle + |1\rangle) \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} (1 + 0) \right|^2 \\ &= \frac{1}{2} \end{aligned}$$

Indeed, as we would expect $|0\rangle$ and $|1\rangle$ in the X basis behave exactly as $|+\rangle$ and $|-\rangle$ do in the Z one.

We will see how the BB84 protocol takes advantage of this fact later in our discussion. The last detail that we want to mention about measurements in non-diagonal bases is that we can actually define unitary operators that allow us to perform measurements in the Z

basis no matter the basis of choice, by first applying some particular unitary operator that creates a “map” between the two bases. For instance, say that we have some vector

$$|v\rangle = \alpha |+\rangle + \beta |-\rangle$$

defined in the X basis, and we want to measure this vector in the Z basis. This can be done by first applying the following operator:

$$U = |0\rangle \langle +| + |1\rangle \langle -|$$

In fact, it holds that

$$\begin{aligned} U|v\rangle &= (|0\rangle \langle +| + |1\rangle \langle -|)(\alpha |+\rangle + \beta |-\rangle) \\ &= |0\rangle \langle +|(\alpha |+\rangle + \beta |-\rangle) + |1\rangle \langle -|(\alpha |+\rangle + \beta |-\rangle) \\ &= \alpha |0\rangle + \beta |1\rangle \end{aligned}$$

We can actually generalize this idea: if we have two bases $\{f_i\}_{i=1}^n$ and $\{g_i\}_{i=1}^n$ an operator that maps each f_i to g_i for all $i \in [n]$ is exactly

$$U_{fg} = \sum_{i=1}^n |g_i\rangle \langle f_i|$$

Interestingly enough, we already know an operator that acts as a map between the X and the Z bases:

$$\begin{aligned} U &= |0\rangle \langle +| + |1\rangle \langle -| \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \right]^\dagger + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot \left[\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \right]^\dagger \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \ 1) + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 \ -1) \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= H \end{aligned}$$

This should not come as a surprise, since we already knew that

$$H|0\rangle = |+\rangle \quad H|1\rangle = |-\rangle$$

5.1.3 The BB84 protocol

The key exchange procedure we will present is called **BB84 protocol**, and it was published in 1984 by Bennett and Brassard [BB14]. The protocol works as follows: suppose that our two usual protagonists Alice and Bob need to share a key quantum-safely. At the beginning, Alice will choose two random binary strings $(4 + \delta)n$ -long — for some $\delta > 0$ sufficiently large — which are usually referred to as a and b . Then, depending on the bits of these two strings she will construct a superposition of states based on the following table:

a_i	b_i	Chosen state
0	0	$ 0\rangle$
1	0	$ 1\rangle$
0	1	$ +\rangle$
1	1	$ -\rangle$

For example, if her two random strings are

$$a = 01101$$

$$b = 00110$$

then she will construct the following superposition

$$|\psi\rangle = |0\rangle \otimes |1\rangle \otimes |-\rangle \otimes |+\rangle \otimes |1\rangle$$

Now, we will assume that Alice and Bob share two communication channels:

- one quantum channel, which can be eavesdropped by a third party Eve that wants to know their shared key
- one public classical *authenticated* channel — in particular Alice and Bob must be sure about the identity of the other

Now that Alice has constructed her superposition $|\psi\rangle$, she will send it to Bob which will receive $\mathcal{E}(|\psi\rangle)$, where \mathcal{E} describes the quantum operation due to the combined effect of the channel's noise and Eve's actions — we will describe what Eve can do later in our discussion.

Bob will then proceed to generate a random string of $(4 + \delta)n$ bits as well, which we will call b' , and based on this very string he will measure the received quantum superposition — in particular, if $b'_i = 0$ he will use the Z base, and if $b'_i = 1$ he will employ the X one. In our example, assuming that Bob generated the random string

$$b' = 10111$$

he will measure something like

$$\text{measure}(|\psi\rangle) = |-\rangle \otimes |1\rangle \otimes |-\rangle \otimes |+\rangle \otimes |+\rangle$$

We observe that the first and the last states randomly collapsed to $|-\rangle$ and $|+\rangle$ respectively because they were measured in the wrong basis — indeed, the original string was $b = 00110$ and $b \oplus b' = 10001$. Bob then tries to reconstruct the original string a based on its b' , thus getting the string

$$a' = 11100$$

When this process is complete, Bob publicly announces that he measured the superposition he received in the authenticated channel to Alice.

After Alice has heard that Bob has measured the state, she can proceed to send b itself *as it is* over the authenticated public channel to Bob — we will see why she is sure that she can perform this operation safely. Through b Bob can then discard all the bits of a' that

were generated through wrong bits of b' — we observe that their remaining bits satisfy $a_i = a'_i$ for all kept indices i . This step is usually called **basis reconciliation**, and the expected number of bits kept by Bob after this step is

$$\mathbb{E}[\text{kept bits}] = \sum_{i=1}^{(4+\delta)n} 1 \cdot \Pr[b_i = b'_i] = \sum_{i=1}^{(4+\delta)n} \frac{1}{2} = \frac{1}{2} \cdot (4 + \delta)n = \left(2 + \frac{\delta}{2}\right)n$$

At this point, Alice and Bob will agree on $2n$ bits to keep from the reconciled string (which can be done again through the public medium) — δ can be chosen sufficiently large so that there are at least $2n$ bits to choose with exponentially high probability.

At this point, the protocol is basically finished, and the last step involves **error correction** which has to take into account both the possible noise of the quantum medium, and the potential actions of Eve. Thus, as final step Alice and Bob agree on a split of their $2n$ bits into 2 sets of n bits (choose UAR), such that half of them will be used as the **shared key**, and the other half are used as *check bits*. In particular, Alice and Bob publicly share the check bits, such that

- if more than t bits disagree, they abort and re-try the protocol from the start
- if less than t bits disagree, the error rate is estimated and used to apply *error correction* algorithms to the key bits — we will not cover the details of the error correction procedures since they are not part of the key distribution protocol itself

5.1.4 Eve's attacks

Now, it's time to discuss the Eve's role in the protocol. Suppose that Eve has access to the quantum channel Alice and Bob are using, and wants to understand the key they are trying to share. At the beginning of the protocol Alice sends her $|\psi\rangle$ which encodes the states she generated through a and b , so what happens if Eve can see this qubit? Due to the No-cloning theorem, she cannot clone $|\psi\rangle$ because in our case we have that

$$S = \{|0\rangle, |1\rangle, |+\rangle, |-\rangle\}$$

and half of the possible pairs are actually non-orthogonal. However, she could theoretically do is intercept $|\psi\rangle$, measure it herself, and send the qubit back to Bob acting as a *man-in-the-middle* — and Bob would have no way to know this actually happened. Nevertheless, nor Bob nor Eve know the sequence of bases Alice chose originally, so the best thing Eve can do is try randomly (exactly as Bob does in the protocol anyway). Hence, fix a state $|\psi\rangle_i$ of the states that constitute $|\psi\rangle$; the following can happen:

- Eve chooses the correct basis for $|\psi\rangle_i$: this means that she does not introduce any disturbance to the state Bob will receive, and Bob still has 50% chance of recovering Alice's original qubit
- Eve chooses the wrong basis for $|\psi\rangle_i$: this means that she introduces some disturbance to the state Bob will receive, in the sense that now Bob has only 25% chance of recovering Alice's original qubit

For instance, suppose that Alice sends $|+\rangle$; if Eve guesses the correct basis it holds that

$$\begin{aligned} \Pr[\text{Bob measures } |+\rangle \mid \text{Eve chooses } X] &= \Pr[\text{Bob measures } |+\rangle \mid \text{Bob chooses } X, \text{Eve sends } |+\rangle] \\ &\quad \cdot \Pr[\text{Bob chooses } X] \\ &\quad \cdot \Pr[\text{Eve sends } |+\rangle \mid \text{Eve chooses } X] \\ &= 1 \cdot \frac{1}{2} \cdot 1 \\ &= \frac{1}{2} \end{aligned}$$

(obviously, all the probabilities are conditioned under the fact that Alice sent $|+\rangle$). Differently, if Eve guesses the wrong basis we have that

$$\begin{aligned} \Pr[\text{Bob measures } |+\rangle \mid \text{Eve chooses } Z] &= \sum_{b \in \mathbb{B}} (\Pr[\text{Bob measures } |+\rangle \mid \text{Bob chooses } X, \text{Eve sends } |b\rangle] \\ &\quad \cdot \Pr[\text{Bob chooses } X] \\ &\quad \cdot \Pr[\text{Eve sends } |b\rangle \mid \text{Eve chooses } Z]) \\ &= \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} \\ &= \frac{1}{4} \end{aligned}$$

Note that 25% is *not* the chances that Bob has to recover $|+\rangle$ *in general*, because that is given by

$$\begin{aligned} \Pr[\text{Bob measures } |+\rangle] &= \sum_{B \in \{X, Z\}} (\Pr[\text{Bob measures } |+\rangle \mid \text{Eve chooses } B] \cdot \Pr[\text{Eve chooses } B]) \\ &= \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{4} \cdot \frac{1}{2} \\ &= \frac{3}{8} \end{aligned}$$

which is still less than $\frac{1}{2}$.

We observe that, on average, with big enough bit strings the chance that Eve correctly chooses each basis can be made exponentially low. Moreover, Eve's actions are exactly the reason why in the last step of the algorithm we perform a thresholded check on the error rate: if the error rate is too high (some noise has to be expected) on average it probably means that someone eavesdropped on the channel.

Is this everything Eve can do? The attack we presented has a very high chance of introducing too much disturbance and being detected by the error rate check step, so for Eve to have some chance of not being detected she needs to **avoid introducing disturbance completely**. The idea is based on the fact that she actually does not need to apply the full No-cloning theorem: suppose that there exists some unitary operator U that on input $|\psi\rangle \otimes |x\rangle$ — for some state $|x\rangle$ — it behaves as follows:

$$U(|\psi\rangle \otimes |x\rangle) = |\psi\rangle \otimes |y\rangle$$

In other words, U leaves $|\psi\rangle$ unchanged and turns $|x\rangle$ into $|y\rangle$. For now, consider $|\psi\rangle$ as 1 single qubit. If such operator exists, Eve could use it in order to try to measure $|y\rangle$ in a later moment and gain some information about $|\psi\rangle$, without ever measuring the latter directly.

This idea seems compelling, however for Eve's attack to be effective U must compute as follows:

$$\begin{aligned} U(|\psi\rangle \otimes |x\rangle) &= |\psi\rangle \otimes |y\rangle \\ U(|\phi\rangle \otimes |x\rangle) &= |\phi\rangle \otimes |y'\rangle \end{aligned}$$

where $|y\rangle$ and $|y'\rangle$ must be **different**. In this way

- U leaves $|\psi\rangle$ unchanged, and the latter can be sent to Bob without anyone noticing
- U behaves differently depending on the input superposition, i.e. $|y\rangle \neq |y'\rangle$, otherwise she cannot distinguish between $|\psi\rangle$ and $|\phi\rangle$ upon measurement — to be clear, this has nothing to do with *entanglement*, in fact for Eve it is sufficient to look at the second qubit and infer what the first must have been based on the fact that $|y\rangle$ and $|y'\rangle$ are distinguishable

Indeed, if such U exists she can recover what the original qubit Alice sent only looking at $|y\rangle$ and using the possible values of the ancilla qubit as “lookup table”. Let's see if she can employ this strategy.

Suppose that Alice sends some qubit which can be either $|\psi\rangle$ or $|\phi\rangle$, where

$$|\psi\rangle, |\phi\rangle \in \{|0\rangle, |1\rangle, |+\rangle, |-\rangle\}$$

Since U must be unitary, by [Proposition 2.8](#) we know that U preserves the scalar product, meaning that

$$\begin{aligned} \langle U(|\psi\rangle \otimes |x\rangle) | U(|\phi\rangle \otimes |x\rangle) \rangle &= \langle \psi \otimes x | \phi \otimes x \rangle \\ \iff \langle \psi \otimes y | \phi \otimes y' \rangle &= \langle \psi \otimes x | \phi \otimes x \rangle \\ \iff \langle \psi | \phi \rangle \langle y | y' \rangle &= \langle \psi | \phi \rangle \langle x | x \rangle \\ \iff \langle \psi | \phi \rangle \langle y | y' \rangle &= \langle \psi | \phi \rangle \end{aligned}$$

We observe that between all the possible choices of pairs of $|\psi\rangle$ and $|\phi\rangle$, half of them are such that $\langle \psi | \phi \rangle \neq 0$, i.e. $|\psi\rangle$ and $|\phi\rangle$ are *non-orthogonal*. This means that we can simplify the last equality even more, obtaining that

$$\begin{aligned} \langle \psi | \phi \rangle \langle y | y' \rangle &= \langle \psi | \phi \rangle \\ \iff \langle y | y' \rangle &= 1 \quad (\langle \psi | \phi \rangle \neq 0) \\ \iff |y\rangle &= |y'\rangle \end{aligned}$$

Once again, through an argument fairly similar of the one we used for the No-cloning theorem, this proves that such an operator U cannot exist, which means that there is no way for Eve to gain any information at all without introducing disturbance.

To be precise, there are more subtle attacks that do employ *quantum entanglement*, such as **optimal intercept–resend tradeoffs**, where Eve applies a unitary operator that *partially entangles* the signal with a probe to trade a small amount of information for a

small disturbance. It can be proven that the BB84 protocol is also resistant against these type of attacks, however this is beyond the scope of our discussion.

Lastly, we observe that BB84 requires Alice to wait before hearing back from Bob that he *actually measured* $|\psi\rangle$. This is to prevent that Alice sends b too early, so that Eve could use the latter to decode $|\psi\rangle$ into the original string a without any issue. Therefore, we require Alice to wait for Bob's measurement so that there is no way for Eve to recover a after looking at b because the original superposition is definitively destroyed — unless she can go back in time!

5.1.5 Bell Inequalities

Imagine we perform the following experiment: there are two parties involved, namely Alice and Bob, and a third party Charlie which prepares two particles. It does not matter how he prepares the particles, the only thing that matters is that he is capable of repeating the experimental procedure which he uses. Once he has completed the preparation procedure, he sends one particle to Alice, and one to Bob.

After Alice receives her particle, she performs a measurement on it. In particular, let's imagine that she has available two different measurement apparatuses, which measure different physical properties that we will label as P_Q and P_R , respectively. For simplicity, we can suppose that the measurements can each have one of two outcomes, namely $+1$ or -1 , and the outcome of measuring property P_Q and P_R are described by two random variables $Q, R \in \{+1, -1\}$ respectively. It is also important to assume that Alice does not know in advance which measurement she will choose to perform, instead when she receives her particle she flips a coin and chooses which property to measure accordingly. Similarly, suppose that Bob is capable of measuring one of two properties, P_S or P_T , and the outcomes of such measurements are also described by random variables $S, T \in \{+1, -1\}$. Again, the choice of the measurement apparatus is random, and we also assume that Alice and Bob do their measurements *at the same time*. This implies that there is no way for Alice's measurement to disturb the result of Bob's measurement (and vice versa) since physical influences cannot propagate faster than light. Interestingly, we can obtain the following result.

Proposition 5.1: Bell inequality

It holds that

$$\mathbb{E}[QS] + \mathbb{E}[RS] + \mathbb{E}[RT] - \mathbb{E}[QT] \leq 2$$

Proof. Let q and r be two outcomes of the random variables Q and R , respectively. Since $q, r \in \{+1, -1\}$, either $q = r$ or $q = -r$, therefore either $q - r = 0$ or $q + r = 0$. For simplicity, let

$$p(q, r, s, t) := \Pr[Q = q, R = r, S = s, T = t]$$

Then, we have that

$$\begin{aligned}
 \mathbb{E}[QS] + \mathbb{E}[RS] + \mathbb{E}[RT] - \mathbb{E}[QT] &= \mathbb{E}[QS + RS + RT - QT] \\
 &= \sum_{q,r,s,t \in \{+1,-1\}} p(q, r, s, t) \cdot (qs + rs + rt - qt) \\
 &= \sum_{q,r,s,t \in \{+1,-1\}} p(q, r, s, t) \cdot [(q+r)s + (r-q)t] \\
 &\leq \sum_{q,r,s,t \in \{+1,-1\}} p(q, r, s, t) \cdot 2 \\
 &\leq 2 \cdot \sum_{q,r,s,t \in \{+1,-1\}} p(q, r, s, t) \\
 &= 2
 \end{aligned}$$

□

This result is also known as the **CHSH inequality**, named after the initials of its four discoverers. Nevertheless, it is generally referred to as the Bell inequality since it is part of a larger set of inequalities known as **Bell inequalities**, named after the work of Bell [Bel64] published in 1964.

By repeating the experiment multiple times, Alice and Bob can determine each term on the LHS of the Bell inequality — for example, after a set of experiments they get a sample of values for Q and S , and by multiplying the results they get multiple estimates of QS which can subsequently be averaged out to get $\mathbb{E}[QS]$. We must underline that in the experiment we described there is *no quantum mechanics involved*: the only thing we did was evaluating expected values and doing calculations with random variables by following a seemingly logical reasoning.

Now, we are going to introduce quantum mechanics in the picture and see what happens with our experiment. Suppose that Charlie prepares a quantum system of two entangled qubits in the Bell state

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

and gives the two qubits to Alice and Bob. To obtain the same exact numbers of the experiment we outlined, we need to consider some properties that Alice and Bob can measure which ultimately yield ± 1 as possible outcomes. Fortunately, we do know such observables and they are the Pauli matrices. In fact, by Postulate 2.2 we know that an observable is a self-adjoint operator, and we already know that all Pauli matrices are self-adjoint. Let's first consider the Z Pauli matrix:

- it's easy to prove that its eigenvalues are exactly $+1$ and -1
- it can also be easily calculated that $|0\rangle$ is an eigenvector of Z associated to $+1$, and $|1\rangle$ is an eigenvector of Z associated to -1 (by solving $Z - \lambda I = 0$ for $\lambda \in \{-1, +1\}$)

This matrix seems to have everything we need for our purposes, so let's set the random variable Q equal to Z . Now, we need to find another observable (i.e. another self-adjoint

operator) to assign to Alice, which also has $+1$ and -1 as eigenvalues and that *does not commute* with Q , meaning that

$$QR \neq RQ$$

This is a crucial detail because we want to express the fact that the order of measurements matters, otherwise the outcomes could be modeled by a single classical random variable. This is easy enough by again turning our attention to the Pauli matrices, in particular we just need to set $R = X$, in fact

- the eigenvalues of X are $+1$ and -1
- $|+\rangle$ is an eigenvector of X associated to $+1$, and $|-\rangle$ is an eigenvector of X associated to -1 (obtained by solving $X - \lambda I = 0$ for $\lambda \in \{-1, +1\}$)
- it can be easily shown that

$$ZX = -XZ$$

The only thing left to define are S and T . For now, we will set them as follows

$$S = \frac{Z - X}{\sqrt{2}} \quad T = \frac{Z + X}{\sqrt{2}}$$

without justifying our choice — we will provide a reason later in our discussion. Most importantly, it can be proven that the eigenvalues of two matrices are still ± 1 .

Our goal now will be to evaluate all the terms of the Bell inequality, and check what quantum mechanics expects as outcome. We are not going into the details of all the calculations — it's a quite tedious task and definitely outside our interests. We will only outline the general idea: for example, to evaluate $\mathbb{E}[QS \mid |\Psi^-\rangle]$ we just need to follow what we described in [Proposition 2.14](#)

Finally, after calculating all 4 terms we end up with the following results:

$$\langle QS \rangle = \frac{1}{\sqrt{2}} \quad \langle RS \rangle = \frac{1}{\sqrt{2}} \quad \langle RT \rangle = \frac{1}{\sqrt{2}} \quad \langle QT \rangle = -\frac{1}{\sqrt{2}}$$

which ultimately yield that

$$\langle QS \rangle + \langle RS \rangle + \langle RT \rangle - \langle QT \rangle = 2\sqrt{2}$$

What? The Bell inequality told us that the LHS could not ever exceed 2, however quantum mechanics predicts that this sum is equal to $2\sqrt{2}$! What is going on?

Short answer: we are not sure. Over the years, multiple experiments have been done to check the prediction of quantum mechanics versus the Bell inequality, and the results are resoundingly in favor of the quantum mechanical outcome. Most notably, in 2022 the Nobel Prize in Physics was awarded to Aspect, Clauser and Zeilinger for having established experimentally the violation of Bell inequalities. In simpler terms, the Bell inequality it *not* obeyed by Nature.

What does this mean? It means that at least one of the assumptions that went into the derivation of the Bell inequality must be incorrect. However, we notice that in the

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experiment we described we relied upon very few assumptions. Among all the various hypotheses on which assumptions are wrong that have been made over the years, two arguments mainly stand out.

1. Assumption of **realism**: this assumes that the physical properties P_Q, P_R, P_S and P_T have definite values Q, R, S and T which exist independent of observation. In fact, our intuition would suggest that every measurement outcome has a definite value *before* it is measured: when we say that

$$Q, R, S, T \in \{+1, -1\}$$

we are also presupposing that the properties to be measured exist before we even perform the measurements. Classically, through measurement we are only looking at definite values that were “already there”.

2. Assumption of **weak locality**: this assumes that measurement performed by Alice does not influence the result of Bob’s measurement. In other words, this assumes that Alice’s choice of measurement cannot change Bob’s values, and vice versa. We want to underline that with this assumption we are not talking about the *outcomes*, only about the *choice* of which measurement apparatus one party selects.

Together, these two assumptions are known as the assumptions of **local realism**. Clearly they seem to be plausible assumptions that match our everyday experience, yet the Bell inequalities show that at least one of the two is incorrect. Most of the physicists believe that the assumption to be dropped is realism, indeed current quantum mechanics believes that there are no values of Q, R, S and T inside the particles and we can only talk about possible measurement outcomes along with their probabilities, but such outcomes do not exist before our measurement. Indeed, this is exactly what we have been assuming from the start: we consider *superposition* of states that collapse only after we have performed our measurement.

To be precise, there is a third possible assumption to consider that we might deem false, which is called **measurement independence**, through which we assume that there exists the possibility of free choice between the measurements that Alice and Bob can perform. However, if this presumption is false, it implies that *free will does not exist* and there are some kind of “hidden variables” that know what settings Alice and Bob will choose in advance. Nevertheless, to this day almost no physicist believes this assumption to be false, so we will only focus on the first two.

As a final note, the choice of S and T was lead by the following bound proved by Tsirelson [Tsi80] in 1980.

Theorem 5.2: Tsirelson bound

Given 4 dichotomic observables A_0, A_1, B_0, B_1 with outcomes $+1$ and -1 such that

$$\forall i, j \in \{0, 1\} \quad A_i B_j = B_j A_i$$

it holds that

$$\langle A_0 B_0 \rangle + \langle A_0 B_1 \rangle + \langle A_1 B_0 \rangle - \langle A_1 B_1 \rangle \leq 2\sqrt{2}$$

The choices for S and T are just the matrices that maximize this bound, given the choices for Q and R .

To this day, it is not known if the world follows either one of them with certainty, but this discrepancy between the classical and the quantum model must imply that the world is not *locally realistic*. Modern quantum mechanics believes in weak locality but not in realism, and interestingly enough such assumption can actually be leveraged in order to design a more quantum-secure key distribution protocol!

Consider again the experiment performed by Alice and Bob, and let \mathcal{A} be the quantity

$$\mathcal{A} := \langle QS \rangle + \langle RS \rangle + \langle RT \rangle - \langle QT \rangle$$

Can an eavesdropper Eve disturb this experiment without any of the two parties involved notice? Recall that the choice of measurements performed by Alice and Bob are executed *randomly*, which means that Eve has no way to know in advance which setting Alice and Bob will pick — not even Alice and Bob do! Therefore, if Eve wants to cheat successfully she must find a way to arrange the context such that she knows all the possible outcomes in advance regardless of the choices of the measurement apparatus performed by the two parties. In other words, Eve must be able to set things up in such a way that she can predict all possible outcomes ahead of time. However, because we are assuming that Nature is weakly local, Eve cannot influence nor Alice's neither Bob's outcomes after they chose which property to measure. This must imply that the only chance she has to cheat is to have some way of “assigning” an outcome to every possible setting *in advance*. This is exactly **realism**, and by Bell inequality any system that is locally realistic must yield a value of $\mathcal{A} \leq 2$.

This is the core idea of the **E91 protocol**, published by Ekert [Eke91] in 1991: suppose that Alice and Bob take a random portion of their qubits and use it in order to compute the quantity \mathcal{A} . Then, if we set Q , R , S and T as we outlined previously we are guaranteed that, without any external disturbance in the setting, the value of \mathcal{A} will be

$$\mathcal{A} \approx 2\sqrt{2}$$

This means that if Alice and Bob measure a value $\mathcal{A} \leq 2$, then their correlations could have come from a locally realistic (and therefore *predetermined*) model. And if their correlations could come from such a model, then Eve could have predicted all outcomes in advance, so their exchange would not be quantum-safe anymore and should be aborted. Hence, by checking the value of \mathcal{A} Alice and Bob can choose to proceed with the exchange of the key or abort their attempt and try again.

5.2 Quantum Error Correction

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