

Lecture notes  
Technologies quantiques, introduction à  
l’algorithmie quantique

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## 1 The computational model: quantum circuits

### 1.1 References

- Nielsen and Chuang - *Quantum computation and quantum information* - [free online pdf](#)
- quantum algorithms with a particular focus on quantum machine learning: <https://quantumalgorithms.org/>
- <https://quantumalgorithmzoo.org/>

## 1.2 qubits

**Definition - quantum computer** A quantum computer is a quantum system composed of  $n$  qubits, whose dynamics can be completely *controlled* by an external observer.

**Definition - qubit** A qubit is a two-level quantum system. The two levels are usually labelled  $|0\rangle$  and  $|1\rangle$ .

The Hilbert space associated to a qubit is therefore:

$$\mathcal{H}_1 = \{\alpha|0\rangle + \beta|1\rangle \quad st \quad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1\}$$

And the Hilbert space associated to a quantum computer, i.e. the space of all possible *states* for a quantum computer is:

$$\begin{aligned} \mathcal{H}_n &= \otimes_{i=1}^n \mathcal{H}_0 \\ &= \left\{ \sum_{i=0}^{2^n-1} a_i |i\rangle \quad st \quad \forall i a_i \in \mathbb{C}, \quad \sum_{i=0}^{2^n-1} |a_i|^2 = 1 \right\} \end{aligned}$$

Above,  $|i\rangle$ , with  $i$  integer denotes the state  $\otimes_{i=1}^n |b_i\rangle$  with  $b_i$  the  $i$ -th<sup>1</sup> bit in the binary decomposition of  $i$ . For small values of  $n$ , the states are typically written with bits directly.

**Definition - state vector** The vector  $[a_i]_{0 \leq i \leq 2^n-1}$  of all amplitudes is typically called the state vector of the quantum computer.

**Remark 1 - dimension** The dimension of the Hilbert space of a quantum computer with  $n$  qubits is therefore  $2^n$ . So about 30 qubits can be hold in RAM on a laptop.

**Remark 2 - initialization** By convention, at the beginning of a quantum computation, the qubits are initialized at  $|0 \dots 0\rangle$ .

**Remark 3 - measure** As usual,  $|a_i|^2$  denotes the probability of observing  $i$  when measuring the state of all qubits. I.e. the probability that qubit 1 is measured in state  $b_1$ , qubit 2 in state  $b_2$ , etc.

## 1.3 Quantum gates

A quantum computer is a *closed* system, thereby following Hamiltonian/unitary dynamics, as per Schrödinger's equation.

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<sup>1</sup>or  $(n-i)$ -th bit, depending on the convention. In this lecture, we work with the convention that  $i = \sum_k b_k 2^k$

**Definition - quantum gates** When using a quantum computer, we modify its state through the application of unitary operations called *quantum gates*. These quantum gates act on the state vector through standard matrix multiplications<sup>2</sup>:

$$|\psi\rangle \xrightarrow[\text{quantum gate } U]{} U|\psi\rangle$$

Quantum gates are almost always *local*, they act non-trivially on a limited number of qubits, while the identity is applied to the other qubits. Mathematically, the overall operation is a *tensor product* of a “small unitary matrix” applied on some qubits, tensored with identity applied on the others. For instance, a 1-qubit gate  $U$  applied on qubit 0 of a system of 3 qubits corresponds to the operation:

$$|\psi\rangle \rightarrow (U \otimes I \otimes I)|\psi\rangle$$

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**Definition - universal gate set** A quantum computer typically comes with a *gate set*, a set of unitary operations involving only a few qubits at a time capable of “generating any other unitary operation”. Universal gate set are universal in light of the Solovay-Kitaev theorem.

**Remark 1 - analogy with classical case** CPU chips (micro-processors) also come with a fixed *instruction set*. These instructions are the only allowed elements in an *assembly* code given to the processor. Chips from different manufacturers typically have different instruction sets. In the case of quantum computers, the different *qubit implementations* (superconducting qubits, atoms, ions) come likewise with different universal gate sets. Conversion rules exist to go from one to another.

**Remark 2 - Usual gates** See Table 1 for a list of usual gates, that quantum computer scientists typically use to write quantum circuit (the notion defined in the next section). This set of usual gates was historically inspired both by what is possible in actual implementations and by what is *practical* to use when designing quantum algorithms.

**Remark 3 - Physically** In practice, gates are implementing by transiently turning *Hamiltonian terms* on/off. Details depend on the qubit implementation.

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<sup>2</sup> $U$  is therefore a  $2^n \times 2^n$  matrix

<sup>3</sup> $I$  is here a  $2 \times 2$  identity matrix, making  $U \otimes I \otimes I$  an  $8 \times 8$  matrix.

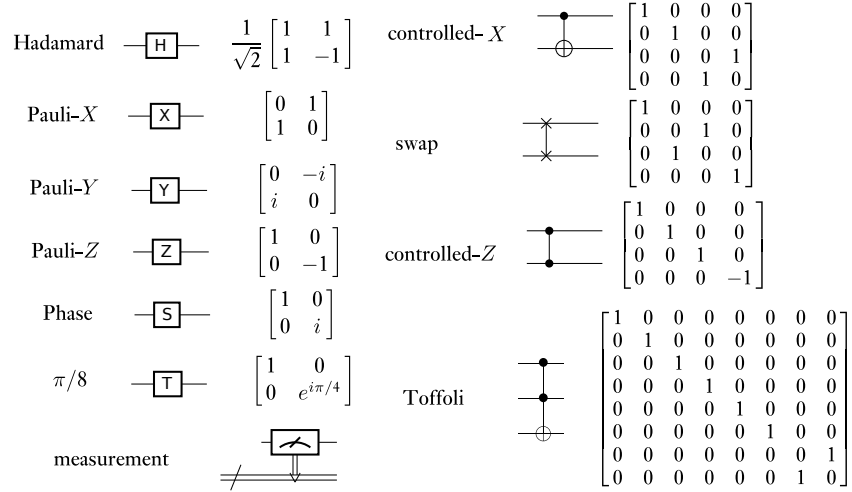
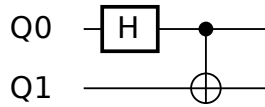


Figure 1: Some usual quantum gates.

## 1.4 Quantum circuits

**Definition - Quantum circuit** A quantum circuit is a graphical representation for a list/sequence of quantum gates applied on  $n$  qubits. As for Boolean circuits in the classical world, *wires* represent qubits. They go through boxes representing gates. We typically refer to the number of gates in a quantum circuit as its *size*

**Example - Bell pair creation** H and then CNOT:



The output state is  $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$

**Example of a fictional basic quantum circuit** and how it manipulates qubits. especially the tensor product operation

## 1.5 Computational model - quantum speedup

**quantum algorithm** The execution of a quantum circuit is the sequential application of all its gates on a quantum computer initialized at  $|0\dots 0\rangle$  followed by the measurement of all qubit. Intermediary measurements may also be applied, and condition the subsequent application of other gates.

**classical complexity** We count the number of elementary operations and upper-bound them asymptotically as a function of the input size<sup>4</sup>.

**quantum complexity** We look at the size of quantum circuits involved in quantum algorithms solving the problem, and asymptotically upperbound it as a function of the input size.

**poly-time quantum and poly-time classical** Poly-time quantum is therefore defined in terms of poly-sized quantum circuits. Poly-time classical has been defined in vaguer terms here, but note that, up to theoretical subtleties beyond the scope of this lecture<sup>5</sup>, classical poly-time complexity could be likewise defined in terms of Boolean circuit size complexity.

- Informally, the question of quantum algorithmics is: which computational problem have a quantum complexity that is asymptotically better than the complexity of any known/possible classical algorithm for the problem ?
- Are there even problems where there is a polynomial quantum algorithm and (as far as we know) only exponential/super-polynomial classical algorithms ?

## 2 Quantum algorithms

### 2.1 by hand example - Deutsch-Josza

From a classical circuit computing a Boolean function, it is fairly easy to get a reversible circuit computing that function. From a reversible circuit, it is easy to get a quantum version using Toffoli-s and CNOTs. This quantum version is usually an oracle, i.e. that does

$$|x\rangle|y\rangle \xrightarrow{O_f} |x\rangle|y \oplus f(x)\rangle$$

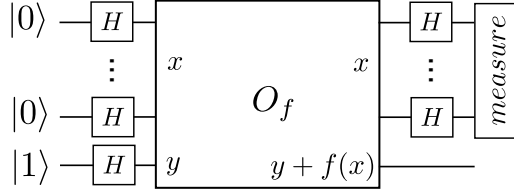
The Deutsch-Josza algorithm solves the following problem:

**Input:** a function  $f : \{0,1\}^n \rightarrow \{0,1\}$ , with the promise that it is either **balanced** ( $|f^{-1}(0)| = |f^{-1}(1)|$ ) or **constant**.

**Task:** decide whether  $f$  is constant or balanced.

<sup>4</sup>number of vertices/edges if the input is a graph, number of bits if the input is a number, number of elements if the input is a list...

<sup>5</sup>circuit “uniformity”



**Classical algorithm** Classically, one needs to compute  $f$  for at least half of the entries plus 1, i.e.  $2^{n-1} + 1$  calls to  $f$  at least.

**Quantum algorithm** Quantumly, one call to the oracle is enough ! With the circuit below.

Let us walk through the steps of the algorithm for  $n = 1$ . In this case, either  $f$  is constant and  $f(0) = f(1) = b$ , or  $f$  is balanced and  $f(0) = b$  while  $f(1) = 1 - b$ . For all binary numbers we write  $\bar{x} = 1 - x$

To start with, Hadamard gates are applied:

$$\begin{aligned} |01\rangle &\xrightarrow{H \otimes H} \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes \left( \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right) \\ &= \left( \frac{|00\rangle + |10\rangle - |01\rangle - |11\rangle}{2} \right) \end{aligned}$$

Then, the oracle, which yields:

$$\frac{|0f(0)\rangle + |1f(1)\rangle - |0\bar{f}(0)\rangle - |1\bar{f}(1)\rangle}{2}$$

Now let us distinguish the two cases:

- if  $f$  is constant, the application of  $H \otimes I$  will yield:

$$\begin{aligned} \frac{|0f(0)\rangle + |1f(1)\rangle - |0\bar{f}(0)\rangle - |1\bar{f}(1)\rangle}{2} &= \frac{|0b\rangle + |1b\rangle - |0\bar{b}\rangle - |1\bar{b}\rangle}{2} \\ &= \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes \left( \frac{|b\rangle - |\bar{b}\rangle}{\sqrt{2}} \right) \\ &\xrightarrow{H \otimes I} |0\rangle \otimes \left( \frac{|b\rangle - |\bar{b}\rangle}{\sqrt{2}} \right) \end{aligned}$$

and therefore 0 is measured.

- if  $f$  is balanced, then  $f(0) = b$  and  $f(1) = \bar{b}$  and:

$$\begin{aligned} \frac{|0f(0)\rangle + |1f(1)\rangle - |0\overline{f(0)}\rangle - |1\overline{f(1)}\rangle}{2} &= \frac{|0b\rangle + |1\bar{b}\rangle - |0\bar{b}\rangle - |1b\rangle}{2} \\ &\xrightarrow{H \otimes I} \frac{\cancel{|0b\rangle} + |1b\rangle + \cancel{|0\bar{b}\rangle} - |1\bar{b}\rangle - \cancel{|0\bar{b}\rangle} - |1\bar{b}\rangle - \cancel{|0b\rangle} + |1b\rangle}{\sqrt{8}} \\ &= |1\rangle \otimes \left( \frac{|b\rangle - |\bar{b}\rangle}{\sqrt{2}} \right) \end{aligned}$$

## 2.2 Quantum Fourier Transform

**Definition** Looking a lot like a quantized version of the Fast Fourier Transform, the definition of the quantum Fourier transform is as such:

$$|j\rangle \xrightarrow{QFT} \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{\frac{2i\pi jk}{2^n}} |k\rangle$$

## 2.3 Phase Estimation

How can such a thing be useful? In fact building block of the blueprint for every quantum algorithms exhibiting a presumed exponential speed-up.

Imagine a unitary operator  $U$  with an eigenvector  $|u\rangle$  and eigenvalue  $e^{2i\pi\phi}$  with  $\phi \in [0, 1[$ . In the case of Shor's algorithm, algorithms for quantum chemistry, quantum linear algebra... *The hard part is computing  $\phi$  for a specific  $U$ .*

The QFT (or rather its inverse) allows to extract  $\phi$  from the following state:

$$\frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2i\pi\phi k} |k\rangle$$

Indeed we can write  $\phi = 0.\phi_0...\phi_{n-1} = \sum_k \frac{\phi_k}{2^k}$ . Which we also write in reverse  $\phi = 0.\tilde{\phi}_{n-1}...\tilde{\phi}_0 = \sum_l \frac{\tilde{\phi}_l}{2^n}$ .

$$\frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2i\pi\phi k} |k\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{\frac{2i\pi k (\sum_l \tilde{\phi}_l 2^l)}{2^n}} |k\rangle$$

Which becomes, when applying an inverse QFT, we get the state  $|\tilde{\phi}_0...\tilde{\phi}_{n-1}\rangle$

But how do we get this state:  $\frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2i\pi\phi k}$  ? Let us write:

$$\begin{aligned} \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2i\pi\phi k} |k\rangle &= \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2i\pi\phi(\sum_l k_l 2^l)} |k\rangle \\ &= \frac{1}{\sqrt{2^n}} \sum_{k_1=0,1} \dots \sum_{k_n=0,1} \prod_l e^{2i\pi\phi k_l 2^l} |k_1 \dots k_n\rangle \\ &= \otimes_{l=0}^{n-1} \left( \frac{|0\rangle + e^{2i\pi\phi 2^l} |1\rangle}{\sqrt{2}} \right) \end{aligned}$$

A state that is almost equal to what we want is  $(H \otimes \dots \otimes H) |0 \dots 0\rangle = \otimes_{l=0}^{n-1} \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right)$ . From it, we need to apply a phase on qubit  $l$  *when it is equal to 1 but not when it is equal to 0*. We can do that with a controlled operation.

We just need to apply  $U^{2^j}$  on  $|u\rangle$ , controlled by qubit  $j$ .

## 2.4 Shor's algorithm and other period-finding algorithms

Finding a non-trivial prime factor of an input integer  $N$  composed of  $n$  bits.

**Best classical algorithm** run-time:  $e^{\Theta(n^{1/3} \log^{2/3} n)}$ .  $\sim$  exponential in the number of bits of  $N$ .

**Shor's algorithm**  $O(\text{poly}(\log(n)))$

**classical part: reduction from factoring to order-finding** I don't know that part: but it reduces the problem to the computation of the period of  $f_a(x) = a^x \bmod N$ .

**quantum part:** **Input:**  $f : \{0,1\}^t \rightarrow \{0,1\}^p$  s.t  $f(x+r) = f(x)$  with  $0 < r < 2^t$

**Task:** compute  $r$ .

**Tool:** a unitary operator  $U$  s.t  $U|x\rangle|y\rangle = |x\rangle|y \oplus f(x)\rangle$

In the case of Shor, we know how to do it.

Computation:

$$\begin{aligned} |0_t\rangle|0_p\rangle &\xrightarrow{H} \frac{1}{\sqrt{2^t}} \sum_{x=0}^{2^t-1} |x\rangle|0_p\rangle \\ &\xrightarrow{U} \frac{1}{\sqrt{2^t}} \sum_{x=0}^{2^t-1} |x\rangle|f(x)\rangle \end{aligned}$$

**Definition pause:** we introduce

$$|\hat{f}(l)\rangle = \frac{1}{\sqrt{r}} \sum_{x=0}^{r-1} e^{\frac{2i\pi lx}{r}} |f(x)\rangle$$



for which the reverse formula is:

$$|f(x)\rangle = \frac{1}{\sqrt{r}} \sum_{l=0}^r e^{\frac{2i\pi lx}{r}} |\hat{f}(l)\rangle$$

Thanks to:  $\sum_{l=0}^r e^{\frac{2i\pi lx}{r}}$  which is equal to  $r$  if  $x$  is a multiple of  $r$  and 0 otherwise.

Going back to our computation:

$$\begin{aligned} \frac{1}{\sqrt{2^t}} \sum_{x=0}^{2^t-1} |x\rangle |f(x)\rangle &= \frac{1}{\sqrt{r}2^t} \sum_{l=0}^r \sum_{x=0}^{2^t-1} e^{\frac{2i\pi xl}{r}} |x\rangle |\hat{f}(l)\rangle \\ &\xrightarrow{Q^{FT^{-1}}} \frac{1}{\sqrt{r}} \sum_{l=0}^r |\tilde{l}/r\rangle |\hat{f}(l)\rangle \end{aligned}$$

Which, if I start again several times and measure, should indeed give me  $r$ .

**applications** Discrete logarithms, Simon's algorithm for Hidden Subgroup problem...

## 2.5 Overview: other algorithms and their speedup

See slide with verbal description

## 3 What you will do in the TP: QPE and VQE for quantum chemistry

see slides.