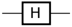
Intervenants

- **Benoît Valiron** (responsable du cours - benoit.valiron@centralesupelec.fr - remplacé par BM)
- **Bertrand Marchand** (bertrand.marchand@lix.polytechnique.fr - TP 1)
- **Simon Martiel** (simon.martiel@atos.net - TP 2)

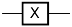
Usual gates

Hadamard



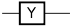
$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

Pauli-X



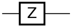
$$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$$

Pauli-Y



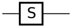
$$\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$$

Pauli-Z



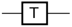
$$\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

Phase



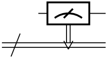
$$\begin{bmatrix}1 & 0\\ 0 & i\end{bmatrix}$$

$\pi/8$

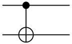


$$\begin{bmatrix}1 & 0\\ 0 & e^{i\pi/4}\end{bmatrix}$$

measurement

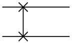


controlled- X



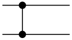
$$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}$$

swap



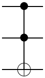
$$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$$

controlled-Z



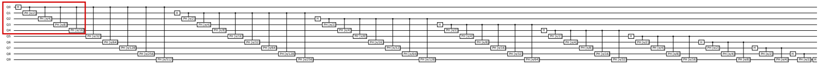
$$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}$$

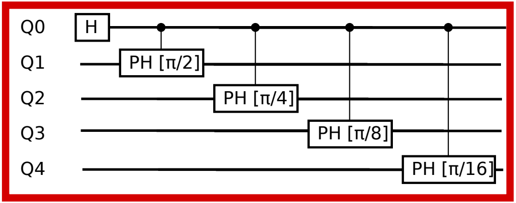
Toffoli



$$\begin{bmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\end{bmatrix}$$

Example of a quantum circuit: QFT





Oracle for SHA256

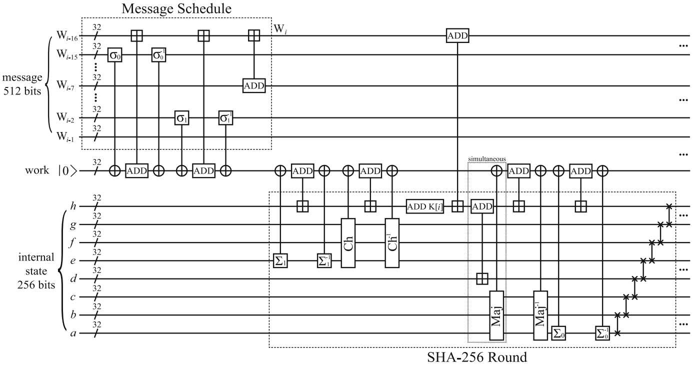


Fig. 10 Reversible circuit for serial implementation of SHA-256 message schedule and round function. The message block consisting of 16 words is recursively updated in place. Note that it is straightforward to make message schedule and round functions work in parallel by expanding the work space. Seven two-qubit gates at the end of round are SWAP gates. The symbol ⊞ is addition modulo 2^{32}

from *Time–space complexity of quantum search algorithms in symmetric cryptanalysis: applying to AES and SHA-2*, Kim et al., 2018.

Overview of quantum algorithms

- **Quantum search algorithms** Use $O(\sqrt{N})$ calls to an oracle O_f to identify elements with $f(x) = 1$ in a list of N elements.
  → generalizations: **quantum walks**
- **QFT-based algorithms**
  - **Shor's algorithm** to factor integers and other **order-finding algorithms**
  - **Quantum chemistry** (and the solving of other Physics/Chemistry problems) through phase estimation.
  - **Quantum linear algebra** and machine learning or other applications.

Quantum phase estimation
-
An example from chemistry

Bertrand Marchand
PhD student @ LIX

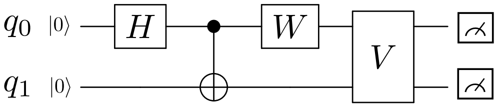
December 3, 2021

Program

1. Some context with these slides.
2. Installation problems ?
3. Your turn. Fill the "quantum_tp_pea.ipynb" according to "TP_instructions.pdf". You will find them in Teams: Files → TP_programmation → TP_kit_phase_estimation
4. Finish it and send it[1] by **Thursday 14 January**.
5. Two important keyboard short-cuts to know: Shift+Enter and Ctrl+Enter.

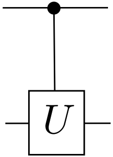
[1] the .ipynb file. Don't forget to save from time to time.

Prequisite: quantum circuits



- qubit: 2-level quantum system ($|0\rangle, |1\rangle$).
  quantum computer = n qubits.
- quantum circuit $\simeq$ quantum program = list of quantum instructions/gates.
- The circuit above computes:
  $|\psi\rangle = V \cdot (W \otimes I) \cdot CNOT_{0\to 1} \cdot (H \otimes I)|00\rangle$

Note: "controlled-gates" means:



$$= \begin{array}{c} \begin{array}{cc|cc} \multicolumn{2}{c|}{q_0 = 0} & \multicolumn{2}{c}{q_0 = 1} \\ q_1,0 & q_1,1 & q_1,0 & q_1,1 \end{array} \\ \left(\begin{array}{cc|c} 1 & 0 & \\ 0 & 1 & (0) \\ \hline \multicolumn{2}{c|}{(0)} & U \end{array}\right) \end{array}$$

Quantum simulation: general motivation

- Efficient numerical simulation quantum phenomena on classical machines seems hard [1].
- Therefore quantum machines might be able to perform classically-intractable computation[2]
- And in particular they should be good at simulating quantum phenomena (e.g simulating QCD, solving condensed-matter problems, computing molecular energies etc.)

—

→ But in practice, how would that work ? What **quantum circuits** would I run on my hypothetical quantum computers to solve these problems ?

[2] basic motivation behind quantum computing research

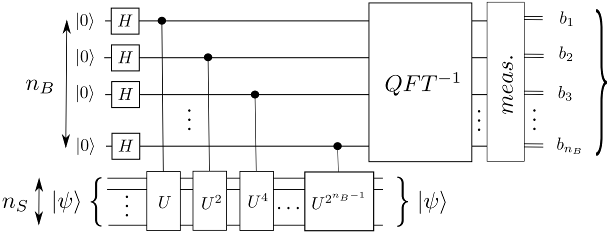
Quantum simulation: more precisely

Most of the time in the potential applications I mentioned (particle phycics, condensed matter, chemistry), the computation consists in **diagonalizing Hamiltonians** and in particular find their **ground state energy**.

You will see in these practical quantum programming sessions the two main frameworks for doing so on a quantum computer:

- **phase estimation** (this week) → the “classic guaranteed-speedup quantum algorithmics approach”.
- **variational quantum algorithms** [2] (next week, in a slightly more “combinatorial optimization”-oriented context) → the “more recent, empirical, practical approach”.

This week's answer: quantum phase estimation



$$\begin{aligned}\phi &= 0.b_1 b_2 b_3 \cdots b_{n_B} \\ &= \sum_k \frac{b_k}{2^k} \\ &= \tfrac{b_1}{2} + \tfrac{b_2}{4} + \cdots\end{aligned}$$

With $|\psi\rangle$ **eigenvector** of U with **eigenvalue** $e^{-2i\pi\phi}$, $(U|\psi\rangle = e^{-2i\pi\phi}|\psi\rangle$, $0 \leq \phi < 1)$

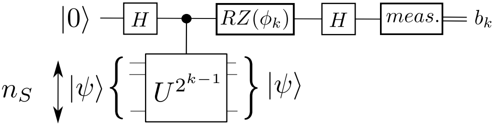
The circuit above allows to compute the n_B most significant bits of ϕ in a **binary decomposition**.

Template for *all* quantum algorithms with **exponential speedup**, both in quantum simulation and other application contexts.

Iterative quantum phase estimation: what we will use

for k in **range**(n_B, 0, -1)[3]:

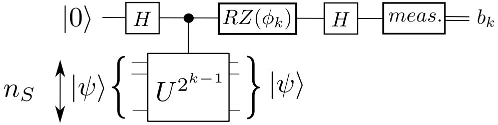
1. compute $\phi_k = 2\pi \cdot \sum_{l=k+1}^{n_B} \frac{b_l}{2^{l-k+1}}$
2. produce and execute the following circuit:



which yields b_k.

With $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and $RZ(\phi_k) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi_k} \end{pmatrix}$

[3] Python style



Recall that $\phi = 0.b_1 \cdots b_{n_B}$ in binary decomposition,
$\phi_k = 2\pi \cdot \sum_{l=k+1}^{n_B} \frac{b_l}{2^{l-k+1}} = 0.0b_{k+1} \cdots b_{n_B}$ and $U|\psi\rangle = e^{-2i\pi\phi}|\psi\rangle$.

Evolution of the system:

$$|0\rangle|\psi\rangle \underset{H}{\rightarrow} \left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)|\psi\rangle = \left(\frac{|0\rangle|\psi\rangle+|1\rangle|\psi\rangle}{\sqrt{2}}\right)$$

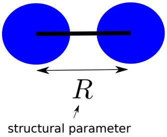
$$\underset{\bullet-U}{\hookrightarrow} \left(\frac{|0\rangle|\psi\rangle+e^{-2i\pi\cdot 2^{k-1}\phi}|1\rangle|\psi\rangle}{\sqrt{2}}\right) = \left(\frac{|0\rangle+e^{-2i\pi\cdot 0.b_k\cdots b_{n_B}}|1\rangle}{\sqrt{2}}\right)|\psi\rangle$$

$$\underset{RZ(\phi_k)}{\hookrightarrow} \left(\frac{|0\rangle+e^{-2i\pi\cdot 0.b_k}|1\rangle}{\sqrt{2}}\right)|\psi\rangle = \left(\frac{|0\rangle+(-1)^{b_k}|1\rangle}{\sqrt{2}}\right)|\psi\rangle \underset{H}{\rightarrow} |b_k\rangle|\psi\rangle$$

Our example: molecular ground state energy calculation

General problem: Given $\mathcal{H}$, electronic structure Hamiltonian of a molecule, we want to compute its ground state energy.

Actually, usually $\mathcal{H}$ depends on some structural/geometric parameters. The purpose is then to compute a *ground state energy landscape* as a function of these parameters. May provide insight on reaction mechanisms [4].



→

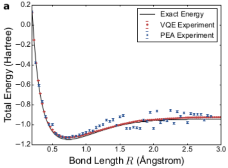
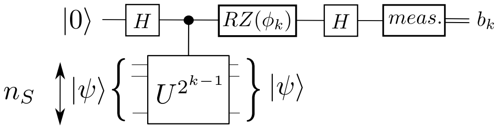


FIG. 3. **Computed H_2 energy curve and errors.** (a) Ene

Our instance: H_2 and its dissociation curve. We will use data from [4], where they solve it on an actual small quantum chip.

[4] Potential futuristic applications: CO_2 capture [3], H_2O cracking...



We will therefore work with:

- $U = e^{-i\mathcal{H}dt}$, for some value of dt to be chosen.
- $|\psi\rangle$ the ground state of H, whose energy E we want to compute.
- we then have $U|\psi\rangle = e^{-iEdt}|\psi\rangle = e^{-2i\pi\frac{Edt}{2\pi}}$

Problem 1: the algorithm only allows us to compute $\phi = \frac{Edt}{2\pi} \text{ mod } [1] \ (\in [0,1])$

Following [5], we will use an *interval guess* $[E_{min}, E_{max}]$ for E. Then $\mathcal{H} \leftarrow \mathcal{H} - E_{min} \cdot I$ ensures $E > 0$ and choosing $dt = \frac{2\pi}{E_{max}}$ ensures $\frac{Edt}{2\pi} < 1$

Other problems

Problem 2 In general we do not have access to the ground state.

→use an **ansatz**[5] with theoretical good overlap with ground state. As suggested in [4], we will use here the Hartree-Fock approxiamtion to our problem, namely $|10\rangle = X \otimes I|00\rangle$

Problem 3 How do we implement $U^{2^k} = e^{-i\mathcal{H}2^k dt}$?

→ usually $\mathcal{H}$ comes as a sum of simpler terms $\sum_l \mathcal{H}_l$ (e.g Pauli products) for which $e^{-i\mathcal{H}_l dt}$ is simple to implement.

→ and use **Trotter's formula** [5]

$$e^{-i\left(\sum_l \mathcal{H}_l\right)dt} \simeq \left(\prod_l e^{-\frac{i\mathcal{H}_l dt}{p}}\right)^p$$

with p integer, as large as possible.

[5] easy-to-prepare approximation

- We will reproduce the curves from [4].
- In this example:
  - $n_S = 2$
  - $H(R) = g_0 I + g_1 ZI + g_2 IZ + g_3 ZZ + g_4 YY + g_5 XX$[6]
  - The coefficients are stored in hamiltonian_data.json
- The purpose is to reproduce

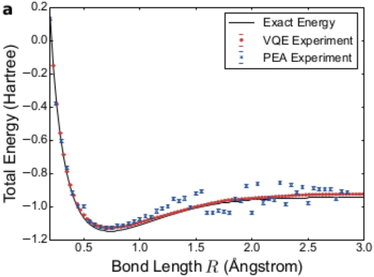


FIG. 3. **Computed H_2 energy curve and errors.** (a) Ene

[6] This Hamiltonian is the output of (1) a conversion from an *electronic structure Hamiltonian* to a *spin Hamiltonian* expressed with Pauli matrices and (2) simplifications leveraging theoretical chemistry knowledge

The programming framework we will use: myqlm

What you need to know:

- quantum circuits are first written as **Program** and then exported as **circuit**.
- A **job** is created from a circuit and sent to a **qpu** (a simulator)
- **AbstractGates** allow to define custom parameterized gates. They will come handy in programming Hamiltonian simulation.
- **QRoutines** allow to program arbitrary parametrized sub-circuits, which are then pluggable anywhere into a larger circuit.
- see the minimal notebook and https://myqlm.github.io/ for more details

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Simulating physics with computers.
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