

Quantum phase estimation

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An example from chemistry

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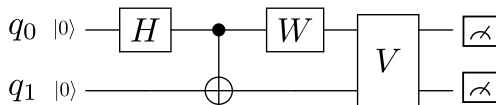
December 10, 2021

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 using the link in the email.
4. Finish it and send it¹ by **next Friday, December 17th**.
5. Two important keyboard short-cuts to know: Shift+Enter and Ctrl+Enter.

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

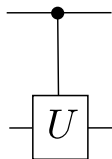
Prerequisite: quantum circuits



- ▶ 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:

$$|\psi\rangle = V \cdot (W \otimes I) \cdot CNOT_{0 \rightarrow 1} \cdot (H \otimes I)|00\rangle$$

Note: “controlled-gates” means:



$=$

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

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 computation²
- ▶ 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 ?

²basic motivation behind quantum computing research

Quantum simulation: more precisely

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

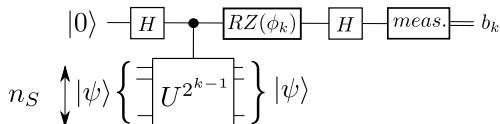
You will see in these practical quantum programming sessions the two main frameworks for doing so on a quantum computer:

- ▶ **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”.

Iterative quantum phase estimation: what we will use

for k in **range**(n_B , 0, -1)³:

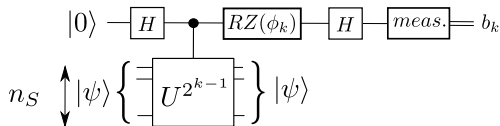
1. compute $\phi_k = 2\pi \cdot \sum_{l=k+1}^{n_B} \frac{b_l}{2^{l-k+1}}$
2. produce and execute the following circuit:



which yields b_k .

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

³Python 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:

$$\begin{aligned}
 |0\rangle|\psi\rangle &\xrightarrow{H} \left(\frac{|0\rangle+|1\rangle}{\sqrt{2}} \right) |\psi\rangle = \left(\frac{|0\rangle|\psi\rangle+|1\rangle|\psi\rangle}{\sqrt{2}} \right) \\
 &\xrightarrow{U} \left(\frac{|0\rangle|\psi\rangle+e^{-2i\pi \cdot 2^{k-1}\phi}|1\rangle|\psi\rangle}{\sqrt{2}} \right) = \left(\frac{|0\rangle+e^{-2i\pi \cdot 0.b_k \cdots b_{n_B}}|1\rangle}{\sqrt{2}} \right) |\psi\rangle \\
 &\xrightarrow{RZ(\phi_k)} \left(\frac{|0\rangle+e^{-2i\pi \cdot 0.b_k}|1\rangle}{\sqrt{2}} \right) |\psi\rangle = \left(\frac{|0\rangle+(-1)^{b_k}|1\rangle}{\sqrt{2}} \right) |\psi\rangle \xrightarrow{H} |b_k\rangle|\psi\rangle
 \end{aligned}$$

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.

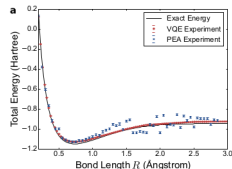
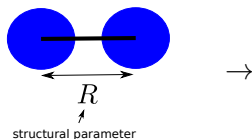
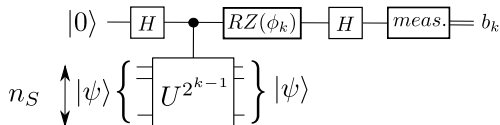


FIG. 3. Computed H₂ energy curve and errors. (a) Ent

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

⁴Potential futuristic applications: CO₂ capture [\[3\]](#), H₂O 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

$$\phi = \frac{Edt}{2\pi} \bmod [1] \ (\in [0, 1])$$

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 approximation 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 $\sum_I \mathcal{H}_I$ (e.g Pauli products) for which $e^{-i\mathcal{H}_I dt}$ is simple to implement.

→ and use **Trotter's formula** [5]

$$e^{-i(\sum_I \mathcal{H}_I)dt} \simeq \left(\prod_I e^{-\frac{i\mathcal{H}_I dt}{p}} \right)^p$$

with p integer, as large as possible.

⁵easy-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

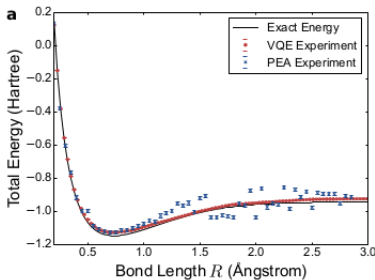


FIG. 3. Computed H_2 energy curve and errors. (a) Enc

⁶This 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



Richard P Feynman.

Simulating physics with computers.

Int. J. Theor. Phys, 21(6/7), 1982.



M Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C Benjamin, Suguru Endo, Keisuke Fujii, Jarrod R McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio, et al.

Variational quantum algorithms.

arXiv preprint arXiv:2012.09265, 2020.



Vera von Burg, Guang Hao Low, Thomas Häner, Damian S Steiger, Markus Reiher, Martin Roetteler, and Matthias Troyer.

Quantum computing enhanced computational catalysis.

arXiv preprint arXiv:2007.14460, 2020.



Peter JJ O'Malley, Ryan Babbush, Ian D Kivlichan, Jonathan Romero, Jarrod R McClean, Rami Barends, Julian Kelly, Pedram Roushan, Andrew Tranter, Nan Ding, et al.

Scalable quantum simulation of molecular energies.

Physical Review X, 6(3):031007, 2016.



James D Whitfield, Jacob Biamonte, and Alán Aspuru-Guzik.
Simulation of electronic structure hamiltonians using quantum computers.

Molecular Physics, 109(5):735–750, 2011.