Quantum simulation

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Outline

Motivation

Simulation of quantum systems is usefull, but is computationally hard!

Motivation

Quantum Simulation was idealized by Feynman[1] and refined by LLoyd[2].

Quote of Richard Feynman:

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly, it's a wonderful problem because it doesn't look so easy."

[1][Richard P Feynman. Simulating physics with computers. International journal of theoretical physics, 21(6-7):467–488, 1982.]
[2][Seth Lloyd. Universal quantum simulators. Science, pages 1073–1078, 1996.]

Motivation

There are many applications for quantum Simulation[1]:

(...)

- Quantum chemistry
- Open quantum systems
- Condensed Matter physics
- Nuclear physics, High-energy physics (Particle physics)
- Cosmology!

Multiple strategies, from "digital" quantum simulations to quantum *analogues*!

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[1][GEORGESCU, Iulia M.; ASHHAB, Sahel; NORI, Franco. Quantum simulation. Reviews of Modern Physics, 2014, 86.1: 153.]

Motivation

Figure: Picture of a black hole

[Alsing, Paul M., Jonathan P. Dowling, and G. J. Milburn. "Ion trap simulations of quantum fields in an expanding universe." Physical review letters 94.22 (2005): 220401.]

The Schrödinger equation

The Schrödinger equation

$$i\hbar \frac{d}{dt}\Psi = H\Psi$$

Classical physics   **Quantum physics**

$$K = \frac{1}{2}mv^2 \qquad\qquad K = \frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

In position basis:

$$i\hbar \frac{d}{dt}\Psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\Psi$$

Solutions for a free particle with $V(x) = 0$, with p being the momentum and E the energy of the system.

$$\Psi(x, t) = Ae^{-i(px - Et)/\hbar}$$

The hydrogen atom

Considering an *Hydrogen* atom (composed by 1 proton and 1 electron):

Figure: The hydrogren atom

Solutions of the Schrödinger equation[1] (3-dimensions):

$$\psi_{nlm}(r, \vartheta, \varphi) = \sqrt{\left(\frac{2}{na_0}\right)\frac{n-l-1!}{2n(n+l)!}}\, e^{-\frac{p}{2}} L_{n-l-1}^{2l+1}(p) Y_l^m(\vartheta, \varphi) \qquad (1)$$

To every combination of n, l, m, denominated **quantum numbers**, corresponds a different solution of the equation.

[1][Y_l^m are the *spherical harmonics* functions and the L_{n-l-1}^{2l+1} are *Laguerre polynomials*]

What is quantum simulation ?

We are usually interested in calculate a properties of interest given Hamiltonians: lowest energy level of an Hamiltonian or other properties of the energy spectra. Many things can be derived from here!

Objective:

- Mimic the **Hamiltonian operator**: Find an $\hat{H}$ such that $H \ket{\Psi} \approx \hat{H} \ket{\Psi}$

- Mimic the **evolution of the Hamiltonian operator**: Find $e^{i\hat{H}}$ such that $e^{i\hat{H}} \ket{\Psi(0)} \approx e^{iH} \ket{\Psi(0)}$!

Very Hard!

- Need to *track* every evolution for each configuration: 2^N. But mainly the **interactions** between them.

Approximating the evolution of an Hamiltonian: A simple example

Evolution of a quantum operator (e^{iHt} is a unitary operator)

$$|\Psi(t)\rangle = e^{iHt} |\Psi(0)\rangle$$

Another way of looking into this (application of the operator over himself until the infinity):

$$e^{iHt} = \lim_{n \to \infty} \left(I + \frac{H}{n} \right)^n$$

Approximation algorithm:

$$|\tilde{\Psi}_0\rangle \leftarrow |\Psi_0\rangle$$
$$j = 0$$
$$while(t_i + j * \Delta t < t_f)$$
$$|\tilde{\Psi_{j+1}}\rangle = U_{\Delta t} |\tilde{\Psi}_j\rangle$$
$$|\Psi(t_f)\rangle = |\tilde{\Psi}_j\rangle$$

Approximating $U_{\Delta t}$

How could be possible to approximate the following Hamiltonian:
$Z \otimes Z \otimes Z$? Evolution is given by: $e^{i(Z \otimes Z \otimes Z)t}$

$$Z \otimes Z \otimes Z = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

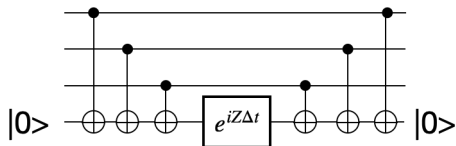# Approximating $U_{\Delta t}$

Evolution of a quantum system:

$$|\Psi_n(t)\rangle = e^{\frac{iE_n t}{\hbar}} |\Psi_n(0)\rangle \qquad (2)$$

Matricial form of $e^{-i(Z\otimes Z\otimes Z)\Delta t}$:

$$e^{i(Z\otimes Z\otimes Z)\Delta t} = \begin{bmatrix} e^{\frac{i\Delta t}{\hbar}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{-\frac{i\Delta t}{\hbar}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{-\frac{i\Delta t}{\hbar}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{\frac{i\Delta t}{\hbar}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-\frac{i\Delta t}{\hbar}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{\frac{i\Delta t}{\hbar}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & e^{\frac{i\Delta t}{\hbar}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-\frac{i\Delta t}{\hbar}} \end{bmatrix};$$

Approximating $U_{\Delta t}$

Resultant circuit:

Diagonal Hamiltonians

If $H = \sum_k^L H_k$ and $\forall_{j \neq i}[H_i, H_j] = 0$ then $e^{iHt} = \prod_i e^{iH_i t}$, for all t.
What if this does not happen ? ($[H_i, H_j] \neq 0$)
A possible solution: diagonalization of the Hamiltonian

$$H_S = T^\dagger H_{S-diag} T \tag{3}$$

The correspondent evolutions reads as follows:

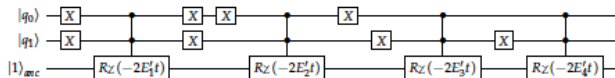$$e^{-iH_S t} = T^\dagger e^{-iH_{S-diag} t} T \tag{4}$$

However T, $T^\dagger$ may be hard to calculate

Diagonal Hamiltonians

Considering a diagonal Hamiltonian:

$$\begin{pmatrix} e^{-iE_1t} & 0 & 0 & 0 \\ 0 & e^{-iE_2t} & 0 & 0 \\ 0 & 0 & e^{-iE_3t} & 0 \\ 0 & 0 & 0 & e^{-iE_4t} \end{pmatrix} \quad (5)$$

A possible circuit to this Hamiltonian reads as follows:

Simulation of the Schrödinger's equation

Schrödinger's equation:

$$i\hbar\frac{d}{dt}\Psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\Psi$$
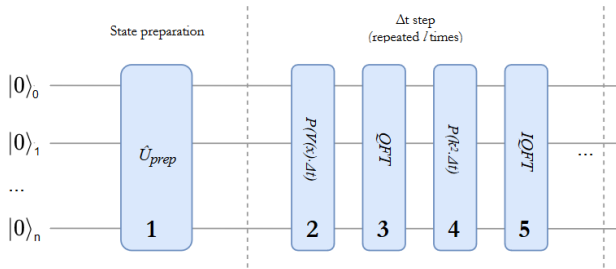
Iterative evolution of Schrödinger's equation:

$$\psi(x_i, t + \Delta t) = e^{-ik^2\Delta t}e^{-iV(x_i)\Delta t}\psi(x_i, t) \qquad (6)$$

The operators $e^{-ik^2\Delta t}$ and $e^{-iV(x_i)}$, relative to velocity and position respectively, do not commute. However the change of basis can be achieved through the Fourier transform.

$$F^{-1}e^{-ik^2\Delta t}Fe^{-iV(x_i)\Delta t} \qquad (7)$$

Simulation of the Schrödinger's equation

[1][Benenti, Giuliano, and Giuliano Strini. "Quantum simulation of the single-particle Schrödinger equation." American Journal of Physics 76.7 (2008): 657-662.]
[2][Afonso Rodrigues, Master thesis]

The Trotter formula

Trotter Formula:

$$\lim_{x \to \infty} (e^{iAt/n} e^{iBt/n})^n = e^{i(A+B)t} \tag{8}$$

$$(e^{iAt/n} e^{iBt/n})^n + \epsilon = e^{i(A+B)t}, \text{ where } \epsilon = \mathcal{O}(\Delta t^2 / N) \text{ and n sufficiently large} \tag{9}$$
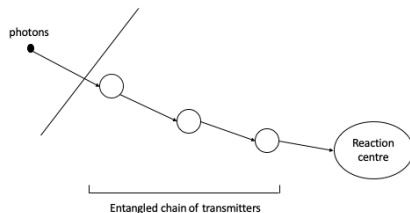
Baker-Campbell-Hausdorff Formula:

$$e^{i(A+B)\Delta t} = e^{iA\Delta t} e^{iB\Delta t} e^{-\frac{1}{2}[A,B]\Delta t^2} + O(\Delta t^3) \tag{10}$$

A case study: Photosynthesis

Photosynthesis: mechanism of collecting and transform the *sunlight*

- Two main phases: energy transport, chemical transformations (reaction centre)
- The energy transport may occur through different mechanics: direct eletrical interaction or photon transport (Förster theory), or even by *coherent effects* and the environment can be relevant (Redfield).

Entangled chain of transmitters

[1][José Diogo Guimarães, Master thesis]

[2][José Diogo Guimarães, Carlos Tavares, Mikhail I. Vasilievsky, "Quantum simulation of photosynthesis", *to be published*]

A case study: Photosynthesis
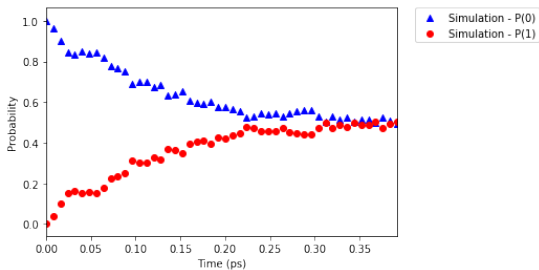
Modeling the molecule chain:

- Site basis: $\sum_{k=0} |k\rangle$
- Each k corresponds to the excitation of the kth site. Transport: Excitation moves from k to $k+1$.

Without environment action:

$$H_S = \sum_m \epsilon_m |m\rangle \langle m| + \sum_{m \neq n} J_{mn} |m\rangle \langle n| \tag{11}$$

where ϵ_m is the site energy of the molecule m and J_{nm} is the coupling strength between the molecules n and m.

A case study: Photosynthesis

What can be calculated with the evolution ?

- The evolution itself: measurement in the appropriate basis
- Calculation of ground states: e.g. Adiabatic computing + Phase estimation

$$H = (1 - t/T)H_i + (t/T)H_p \tag{12}$$

Calculation of the ground state with the Variational quantum eigensolver

This variational quantum eigensolver allows the calculation of the ground state of a system

Given a state of the shape:

$$|\Psi\rangle = \lambda_1 |\Psi_1\rangle + \lambda_2 |\Psi_2\rangle + \ldots + \lambda_n |\Psi_n\rangle \tag{13}$$

The objective is to find:

$$\min \left(H |Psi\rangle \right) \tag{14}$$

Hamiltonian Formalism

The hamiltonians describe the total energy of systems, which contains the operations associated with the kinetic and potential energies.

Generic formula:

$$H = K + V = -\frac{\hbar}{2m}\nabla^2 + V$$

For the majority of chemistry systems a Fermionic[1] Hamiltonian is enough. Total Fermionic Hamiltonian considering all interactions:

$$H = -\sum_{i=1}^{N}\frac{1}{2}\nabla_i^2 - \sum_{A=1}^{M}\frac{1}{2M_A}\nabla_{A^2} - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{r_{BA}}$$

[1]Fermions are subatomic particles, such as an electron/proton, which has half-integral spin and follows the Fermi-Dirac statistics.

[2] Components (left to right) - kinectic energy electrons; kinectic energy of nuclei; electric attraction nuclei - electrons; electric repulsion electrons; electric repulsion nuclei

[Attila Szabo and Neil S Ostlund. Modern quantum chemistry: introduction to advanced electronic structure theory. Courier Corporation, 2012.]

Hamiltonian Formalism

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Generic formula:

$$H = K + V = -\frac{\hbar}{2m}\nabla^2 + V$$

For the majority of chemistry systems a Fermionic[1] Hamiltonian is enough. Electronic hamiltonian after applying Born-Oppenheimer approximation:

$$H_{elec} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}}$$

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[2] Components (left to right) - kinectic energy electrons; kinectic energy of nuclei; electric attraction nuclei - electrons; electric repulsion electrons; electric repulsion nuclei

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Orbitals

When dealing with Fermionic systems, *spin* plays an important role (Pauli exclusion principle) (χ - Orbital, solution for the wave equation $+$ spin)

$$\Psi(\chi_1, \chi_2) = -\Psi(\chi_2, \chi_1) \tag{15}$$

The Hamiltonians have to act over the orbitals? Which orbitals?

$$H\ket{\Psi} = E\ket{\Psi}$$

Solution: Use wave function approximations (here STO3G functions are used).

$$\phi_{1s}^{\mathrm{STO-3G}}(\zeta, \mathbf{r}) = c_1\left(\frac{2\alpha_1}{\pi}\right)^{\frac{3}{4}} e^{-\alpha_1 r^2}$$
$$+ c_2\left(\frac{2\alpha_2}{\pi}\right)^{\frac{3}{4}} e^{-\alpha_2 r^2} + c_3\left(\frac{2\alpha_3}{\pi}\right)^{\frac{3}{4}} e^{-\alpha_3 r^2}. \tag{16}$$

Second Quantization

The Second Quantization is an alternative formalism for specifying Hamiltonians.

- Creation and annihilation operators (allows systems with variable dimension)

$$a_i^\dagger \left| \chi_1 \chi_2 \ldots \chi_n \right\rangle = \left| \chi_i \chi_1 \chi_2 \ldots \chi_n \right\rangle ; a_i \left| \chi_i \chi_1 \chi_2 \ldots \chi_n \right\rangle = \left| \chi_1 \chi_2 \ldots \chi_n \right\rangle \tag{17}$$

- The creation an annihilation operators already encompass the necessary symmetry of the wave equations

$$a_\alpha \, a_\beta^\dagger + a_\alpha^\dagger \, a_\beta = \delta_{\alpha\beta} \,. \tag{18}$$

[Dirac, Paul Adrien Maurice. The principles of quantum mechanics. No. 27. Oxford university press, 1981]

Second Quantization

Hamiltonian:

$$H = H_1 + H_2 = \sum_{\alpha,\beta=0}^{M-1} \tau_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta=0}^{M-1} \mu_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\gamma^\dagger a_\delta a_\beta$$

where

$$\tau_{\alpha\beta} = \int dx_1 \psi_\alpha^*(x_1) \left(\frac{-\nabla^2}{2} + \sum_i \frac{Z_i}{|r_{i1}|} \right) \psi_\beta(x_1)$$

and

$$\mu_{\alpha\beta\gamma\delta} = \int dx_1 dx_2 \psi_\alpha^*(x_1) \psi_\beta(x_1) \left(\frac{1}{|r_{12}|} \right) \psi_\gamma^*(x_2) \psi_\delta(x_2)$$

where $\tau_{\alpha\beta}$ and $\mu_{\alpha\beta\gamma\delta}$ are matrix/operator coefficients.

Integeral calculation

As it seems obvious we are not able to calculate the whole set of integrals, we have to choose a subset of the basis set, i.e. one that contains the ground state. There are several methods to the approximation of these integrals: MO-LCAO. It is possible to refine the first approximation with the Hartreee-Fock method.
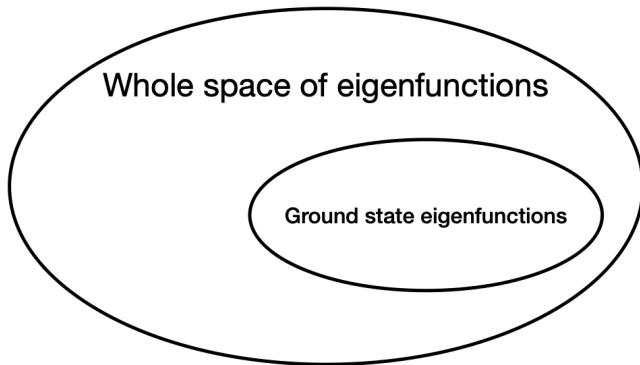

Figure:

Jordan-Wigner Transformation

Has the purpose to map fermions into qubits.

σ^- represents the spin-lowering operator and σ^+ the spin-raising operator, which can be written in terms of Pauli operator:

$$\sigma^- = \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\sigma^+ = \frac{1}{2}(\sigma_x - i\sigma_y) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Lowering and raising operators over sets of qubits:

$$a_j^\dagger = 1^{\otimes j-1} \bigotimes \sigma^- \bigotimes \sigma^{Z \otimes N-j-1}$$

$$a_j = 1^{\otimes j-1} \bigotimes \sigma^+ \bigotimes \sigma^{Z \otimes N-j-1}$$

[James D Whitfield, Jacob Biamonte, and Alán Aspuru-Guzik. Simulation of electronic structure hamiltonians using quantum computers. Molecular Physics, 109(5):735–750, 2011.]

Quantum Circuit

Description	Second Quantization[a]	Pauli representation
Number Operator	$h_{pp}a_p^\dagger a_p$	$\frac{h_{pp}}{2}(\mathbf{1}_p - \sigma_p^z)$
Excitation Operator	$h_{pq}a_p^\dagger a_q + h_{qp}a_q^\dagger a_p$	$\frac{1}{2}\left(\bigotimes_{k=q+1}^{p-1}\sigma_k^z\right)\left(\begin{array}{c}\Re\{h_{pq}\}(\sigma_q^x\sigma_p^x + \sigma_q^y\sigma_p^y)\\ +\Im\{h_{pq}\}(\sigma_q^y\sigma_p^x - \sigma_q^x\sigma_p^y)\end{array}\right)$
Coulomb Operators	$h_{pqqp}a_p^\dagger a_q^\dagger a_q a_p$	$\frac{h_{pqqp}}{4}\left(\mathbf{1} - \sigma_p^z - \sigma_q^z + \sigma_p^z\sigma_q^z\right)$
Number with[b] Excitation Operator	$h_{pqqr}a_p^\dagger a_q^\dagger a_q a_r + h_{rqqp}a_r^\dagger a_q^\dagger a_q a_p$	$\left(\bigotimes_{k=r+1}^{p-1}\sigma_k^z\right)\left[\left(\begin{array}{c}\Re\{h_{pqqr}\}(\sigma_r^x\sigma_p^x + \sigma_r^y\sigma_p^y)\\ +\Im\{h_{pqqr}\}(\sigma_r^y\sigma_p^x - \sigma_r^x\sigma_p^y)\end{array}\right) - \sigma_q^z\left(\begin{array}{c}\Re\{h_{pqqr}\}(\sigma_r^x\sigma_p^x + \sigma_r^y\sigma_p^y)\\ +\Im\{h_{pqqr}\}(\sigma_r^y\sigma_p^x - \sigma_r^x\sigma_p^y)\end{array}\right)\right]$
Double Excitation Operator	$h_{pqrs}a_p^\dagger a_q^\dagger a_r a_s + h_{srqp}a_s^\dagger a_r^\dagger a_q a_p$	$\left(\bigotimes_{k=s+1}^{r-1}\sigma_k^z\right)\left(\bigotimes_{k=q+1}^{p-1}\sigma_k^z\right)\left(\begin{array}{c}\frac{\Re\{h_{pqrs}\}}{8}\left(\begin{array}{c}\sigma_s^x\sigma_r^x\sigma_q^x\sigma_p^x - \sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^y + \sigma_s^x\sigma_r^y\sigma_q^x\sigma_p^y\\ +\ \sigma_s^y\sigma_r^x\sigma_q^x\sigma_p^y + \sigma_s^y\sigma_r^x\sigma_q^y\sigma_p^x - \sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^x\\ +\ \sigma_s^x\sigma_r^y\sigma_q^y\sigma_p^x + \sigma_s^y\sigma_r^y\sigma_q^y\sigma_p^y\end{array}\right)\\ +\frac{\Im\{h_{pqrs}\}}{8}\left(\begin{array}{c}\sigma_s^y\sigma_r^x\sigma_q^x\sigma_p^x + \sigma_s^x\sigma_r^y\sigma_q^x\sigma_p^x - \sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^x\\ -\ \sigma_s^x\sigma_r^y\sigma_q^y\sigma_p^y - \sigma_s^y\sigma_r^x\sigma_q^y\sigma_p^y + \sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^y\\ +\ \sigma_s^y\sigma_r^y\sigma_q^y\sigma_p^x + \sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^x\end{array}\right)\end{array}\right)$

Figure: Summary of operators representation

In fact there are more efficient quantum circuit encodings:parity encoding.

[James D Whitfield, Jacob Biamonte, and Alán Aspuru-Guzik. Simulation of electronic structure hamiltonians using quantum computers. Molecular Physics, 109(5):735–750, 2011.]

Quantum Circuit

General shape of the Hamiltonian's circuit after the application of the Jordan-Wigner transform (or similar);

$$H = \sum_{i;\, q} h_q^i \sigma_i^{(q)} + \sum_{i_1, i_2;\, q_1, q_2} h_{q_1, q_2}^{i_1, i_2} \sigma_{i_1}^{(q_1)} \otimes \sigma_{i_2}^{(q_2)} + \cdots \tag{19}$$

h - coefficients q - qubit index i - type of pauli gate (x, y, z)
There are tools to do these transformations available in IBM Q, or quipper

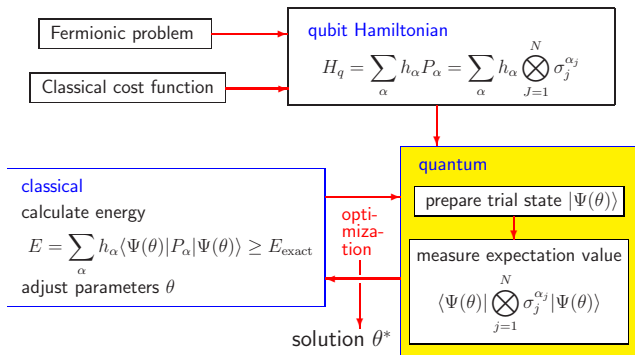# Variational Quantum Eigensolver

Figure:

[Nikolaj Moll, Panagiotis Barkoutsos, Lev S Bishop, Jerry M Chow, Andrew Cross, Daniel J Egger, Stefan Filipp, Andreas Fuhrer, Jay M Gambetta, Marc Ganzhorn, et al. Quantum optimization using variational algorithms on near-term quantum devices. arXiv preprint arXiv:1710.01022, 2017.]

Quantum Expected value Estimation (QEE)

Calculation of the expected value of the Hamiltonian

$$
\begin{aligned}
\langle H \rangle &= \langle \Psi | H | \Psi \rangle \\
&= \sum_{i;\, q} h_q^i \langle \sigma_i^{(q)} \rangle + \sum_{\substack{i_1, i_2; \\ q_1, q_2}} h_{q_1, q_2}^{i_1, i_2} \langle \sigma_{i_1}^{(q_1)} \otimes \sigma_{i_2}^{(q_2)} \rangle + \cdots
\end{aligned}
\tag{20}
$$

Table: Comparison of resources needed for two methods, *Quantum phase estimation* and QEE. M: the number of independent terms of the Hamiltonian approximation, p: the precision chosen, $O(...)$: *assymptotic* lower bound of the associated resource function.

Method	Number of state preparations	Coherence time	Number of steps
QEE	$O(M)$	$O(1)$	$O(|h_{max}|^2 M p^{-2})$
QPE	$O(1)$	$O(p^{-1})$	$O(p^{-1})$

Preparation of trial states

It is necessary a *vaccum* state. Obtainable for instance by the Hartree-Fock method. However, it is just an approximation to the ground state.

$$|\Psi_0\rangle = \prod_{\alpha}^{N} a_{\alpha}^{\dagger}|\text{vac}\rangle \, ,$$

The trial states can be obtained by the application of a parameterizable operator $\hat{U}(\overrightarrow{\theta})$, where $\overrightarrow{\theta}$, is a vector of *real* numbers.

$$|\Psi(\overrightarrow{\theta})\rangle = \hat{U}(\overrightarrow{\theta})|\Psi_0\rangle \, , \tag{21}$$

Example of an ansatz: the UCC

$$|\Psi(\overrightarrow{\theta})\rangle = e^{\hat{T}(\overrightarrow{\theta}) - \hat{T}^{\dagger}(\overrightarrow{\theta})}|\Psi_0\rangle \, . \tag{22}$$

Preparation of trial states

Here $\hat{T}$ is an operator representing excitations from occupied to unoccupied states (labeled below by Greek and Latin indices, respectively), composed of hierarchical terms,

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots ,$$

corresponding to n-particle excitations, namely,

$$\hat{T}_1(\overrightarrow{\theta}) = \sum_{\alpha,a} \theta_\alpha^a a_a^\dagger a_\alpha , \tag{23}$$

$$\hat{T}_2(\overrightarrow{\theta}) = \frac{1}{2} \sum_{\alpha,\beta;\, a,b} \theta_{\alpha\,\beta}^{a\,b} a_a^\dagger a_b^\dagger a_\alpha a_\beta , \tag{24}$$

$$\dots$$

The optimization method

Generally an optimization method is constituted by two steps: evaluation of a solution and the search for other solutios:

Evaluation of the function in the VQE method:

$$E[\Psi(\overrightarrow{\theta})] = \frac{\langle \Psi(\overrightarrow{\theta})|H|\Psi(\overrightarrow{\theta})\rangle}{\langle \Psi(\overrightarrow{\theta})|\Psi(\overrightarrow{\theta})\rangle} . \tag{25}$$

The search for new solutions will made by a classical method for the real parameters $\overrightarrow{\theta}$, example: Cobyla method, Gradient descent.
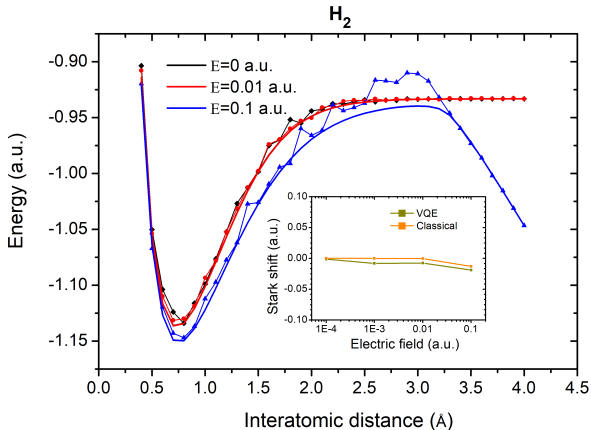
IBM

Table: The set of technical parameters used for quantum calculations.

parameter	value
shots[a]	4096
Max. number of iterations of Cobyla	15000
Max. number of iterations of PySCF	5000
optimization level	3
mapping method	Jordan-Wigner
QISkit version	0.13.0

[a]number of times the execution of circuits is to be performed due to the stochastic nature of quantum computers
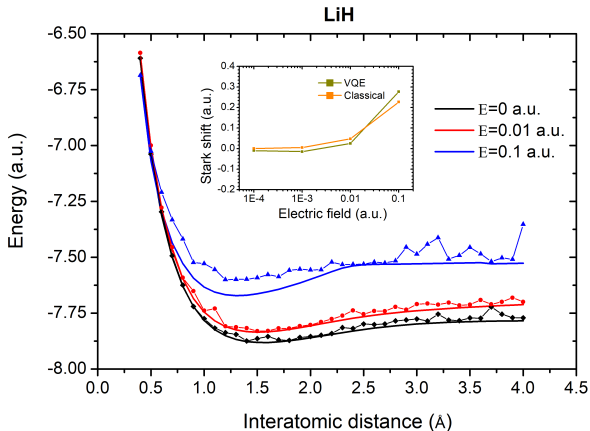
Results - H_2 molecule

Figure: Dissociation curve of H_2 molecule, as calculated with a classical solver (full lines) and with the VQE (symbols connected by lines), for several values of the external electric field $\mathbb{E}$ marked by color. The Stark effect (i.e. the shift of the minimum energy with electric field) is shown in the inset.

Results - LiH molecule

[Carlos Tavares, Sofia Oliveira, Vitor Fernandes, Andrei Postnikov, Mikhail I. Vasilevskiy. Quantum simulation of the ground–state Stark effect in small molecules: A case study using IBM Q. *to be published*, 2020 (?).]

Expectations for the Future

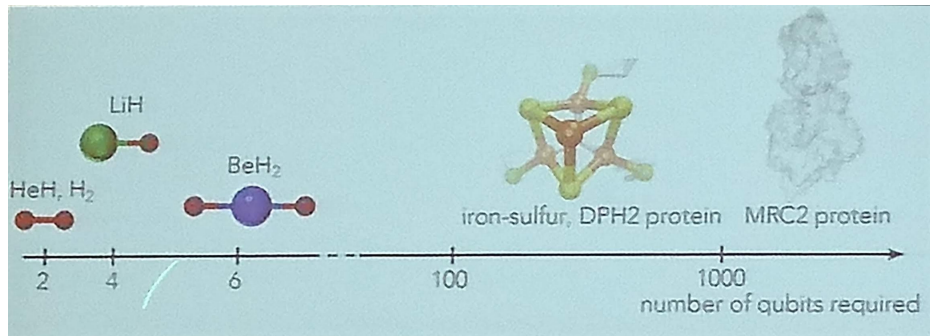So where do Quantum computation stands now?

Figure: Number of Qubits per molecule - IBM Research

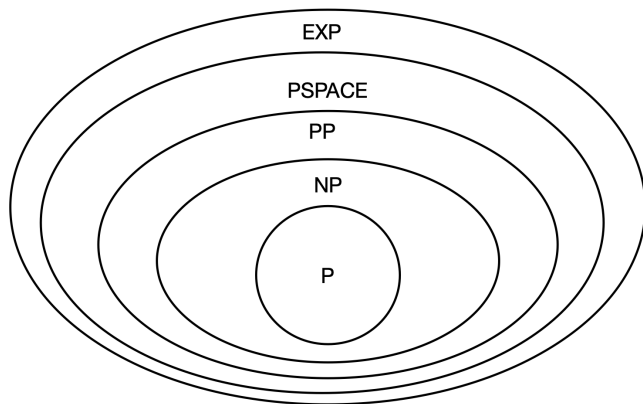# Expectations for the Future

So where do we stand now?

Chemistry constitutes a natural field of application for quantum mechanics. We are interested in applying this methodology to study physical phenomena on the effects of physical fields over molecules.

It also seems feasisble to study simplified models of biology. Quantum physics is quite relevant in many biological phenomena:
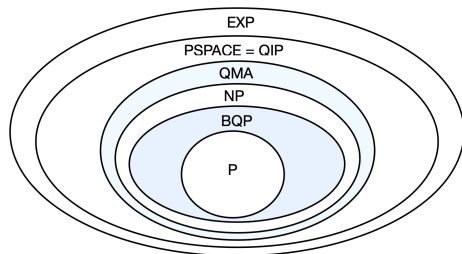
- photosynthesis, vision, smell...
- Origins of life? Conscioussness?[1]

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[1][Schrödinger, E. (1992). What is life?: With mind and matter and autobiographical sketches. Cambridge University Press.]

Quantum computational complexity

Quantum computational complexity

$$P \subseteq BQP \subseteq NP \subseteq QMA \subseteq PSPACE \equiv QIP \subseteq EXP$$

BQP class - All computational problems efficiently solvable by quantum computers: Shor algorithm

Quantum computational complexity

QMA class - is the quantum analogous of the NP class. The complexity of these problems are studied in the field of **Hamiltonian complexity**

- Problems: QC-SAT, QC-Circuit, k-Local Hamiltonian, Density matrix consistency
- Finding the Ground State is hard even for a quantum computer, and in fact many classical optimization problems (NP-HARD) can be reduced to a ground state problem

QIP class - A generalization of the QMA class, where an unbounded of number of interactions between the prover and verifier are allowed

Quantum computational complexity: exotic physics

Post BQP ≡ PP - Very powerful computational class, possible if physics had post-selection: if one can restrict the probabilities in the result state.

Quantum computation with CTC's ≡ PSPACE - Computations possible in a quantum physics with closed timelike curves: all computable functions with Polynomial resources are efficient.
Both are types of quantum physics with non-linearities.

Questions?