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*!

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

Motivation
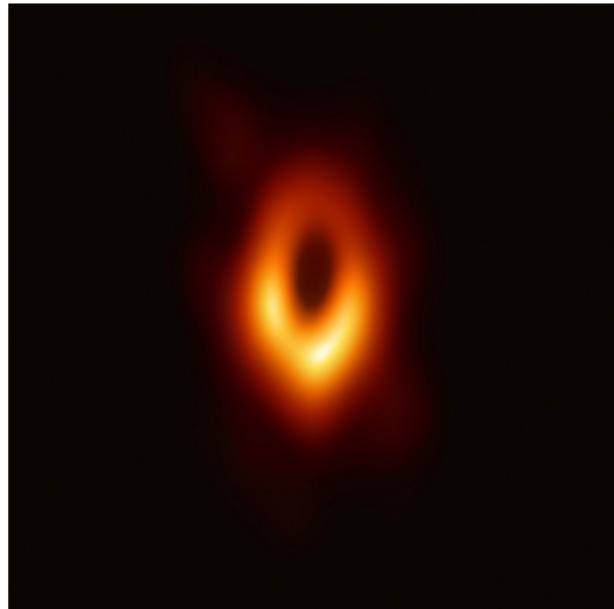
Figure: Picture of a black hole

[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**

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

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*]

The Schrödinger equation - interpretation

Which of those equations capture the behaviour of a system? Answer: A superposition of them?

- A quantum number refers to a physical characteristic of the system: energy, momentum, braiding...
- One (of several) problems: the **Measurement problem**!

Quantum mechanics is captured in the Hilbert space formalism:

- States $|\Psi\rangle$
  - ▶ States are vectors in the Hilbert space, spanned by an orthogonal basis $\langle\Psi_1|\Psi_2\rangle = 0$:

$$|\Psi\rangle = \lambda_1 |\Psi_1\rangle + \lambda_2 |\Psi_2\rangle + \ldots + \lambda_n |\Psi_n\rangle$$

  - ▶ **Superposition principle**: every superposition of the base vectors is a possible state of the system.

The Schrödinger equation - interpretation

- ▶ **Börn interpretation**: Probabilistic interpretation! Probability of obtaining $|\Psi_x\rangle$ given by $|\lambda_x|^2$ and $\sum_x |\lambda|^2 = 1$
- Operators $O|\Psi\rangle$
  - ▶ Operators are linear operators/matrix on the Hilbert space.

$$\begin{bmatrix} \langle\Psi_1|O\Psi_1\rangle & \langle\Psi_2|O\Psi_1\rangle & \dots & \langle\Psi_n|O\Psi_1\rangle \\ \langle\Psi_1|O\Psi_2\rangle & \langle\Psi_2|O\Psi_2\rangle & \dots & \langle\Psi_n|O\Psi_2\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\Psi_1|O\Psi_n\rangle & \langle\Psi_2|O\Psi_n\rangle & \dots & \langle\Psi_n|O\Psi_n\rangle \end{bmatrix} \tag{2}$$

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

Very Hard!

- Need to *track* every evolution for each configuration: 2^N

What is quantum simulation ?

Classical computational methods: Monte Carlo Simulation, Density Functional theory, Variational methods...

Quantum computational methods:

| Mimic the evolution | Mimic the Hamiltonian |

| Digital quantum simulation | | Analog quantum simulation |

| Adiabatic method | Phase estimation method | Quantum variational method |

| Trotter method | Jordan-Wiger transform |

Approximating the evolution of an Hamiltonian

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: $e^{i(Z \otimes Z \otimes Z)t}$

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 ? ($[H_i, H_j] \neq 0$)
Trotter Formula:

$$\lim_{x \to \infty} (e^{iAt/n} e^{iBt/n})^n = e^{i(A+B)t} \tag{3}$$

Baker-Campbell-Hausdorff Formula:

$$e^{i(A+B)\Delta t} = e^{iA\Delta t} e^{iB\Delta t} e^{-\frac{1}{2}[A,B]\Delta t^2} + O(\Delta t^3) \tag{4}$$

Quantum computational complexity

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

The complexity of these problems are studied in the field of **Hamiltonian complexity**

- Class QMA is the quantum analogous of the NP class
- Problems: QC-SAT, QC-Circuit, k-Local Hamiltonian, Density matrix consistency

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.]

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

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

[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

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Second Quantization

When dealing with Fermionic systems, *spin* plays an important role (Pauli exclusion principle):

$$\Psi(\chi_1, \chi_2) = -\Psi(\chi_2, \chi_1) \tag{5}$$

χ - Orbital, solution for the wave equation + spin, for a particle in the system

The Second Quantization is an alternative formalism for specifying Hamiltonians.

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

$$a_i^\dagger \left| \chi_1 \chi_2 \dots \chi_n \right\rangle = \left| \chi_i \chi_1 \chi_2 \dots \chi_n \right\rangle ; a_i \left| \chi_i \chi_1 \chi_2 \dots \chi_n \right\rangle = \left| \chi_1 \chi_2 \dots \chi_n \right\rangle \tag{6}$$

[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.
What are the ψs..?

- In our case, it has used STO-3G wavefunctions (ψ).

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	$h_{pqqp}a_p^\dagger a_q^\dagger a_q a_p$	$\frac{h_{pqqp}}{4}\left(1 - \sigma_p^z - \sigma_q^z + \sigma_p^z\sigma_q^z\right)$
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	$h_{pqrs}a_p^\dagger a_q^\dagger a_r a_s + h_{srqp}a_s^\dagger a_r^\dagger a_q a_p$	$\left(\bigotimes_{k=s+1}^{r-1}\sigma_k^z\right)\left(\bigotimes_{k=q+1}^{p-1}\sigma_k^z\right)\left(\begin{array}{c}\frac{\Re\{h_{pqrs}\}}{8}\left(\begin{array}{c}\sigma_s^x\sigma_r^x\sigma_q^x\sigma_p^x - \sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^y + \sigma_s^x\sigma_r^y\sigma_q^x\sigma_p^y\\ +\ \sigma_s^y\sigma_r^x\sigma_q^x\sigma_p^y + \sigma_s^y\sigma_r^x\sigma_q^y\sigma_p^x - \sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^x\\ +\ \sigma_s^x\sigma_r^y\sigma_q^y\sigma_p^x + \sigma_s^y\sigma_r^y\sigma_q^y\sigma_p^y\end{array}\right)\\ +\frac{\Im\{h_{pqrs}\}}{8}\left(\begin{array}{c}\sigma_s^y\sigma_r^x\sigma_q^x\sigma_p^x + \sigma_s^x\sigma_r^y\sigma_q^x\sigma_p^x - \sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^x\\ -\ \sigma_s^x\sigma_r^y\sigma_q^y\sigma_p^y - \sigma_s^y\sigma_r^x\sigma_q^y\sigma_p^y + \sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^y\\ +\ \sigma_s^y\sigma_r^y\sigma_q^y\sigma_p^x + \sigma_s^x\sigma_r^x\sigma_q^x\sigma_p^y\end{array}\right)\end{array}\right)$

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.]

Techniques

In quantum chemistry one may be interested in many different calculations: thermal rates, phase diagrams, **ground state**

There are many methods to calculate the Ground State in chemistry, such as the Adiabatic Computation (based on the Hamiltonian evolution), the Phase Estimation Algorithm (based on Hamiltonian evolution) and the **Variational Quantum Eigensolver (based just on the Hamiltonian action)**.

It was used the last one.

Variational Quantum Eigensolver
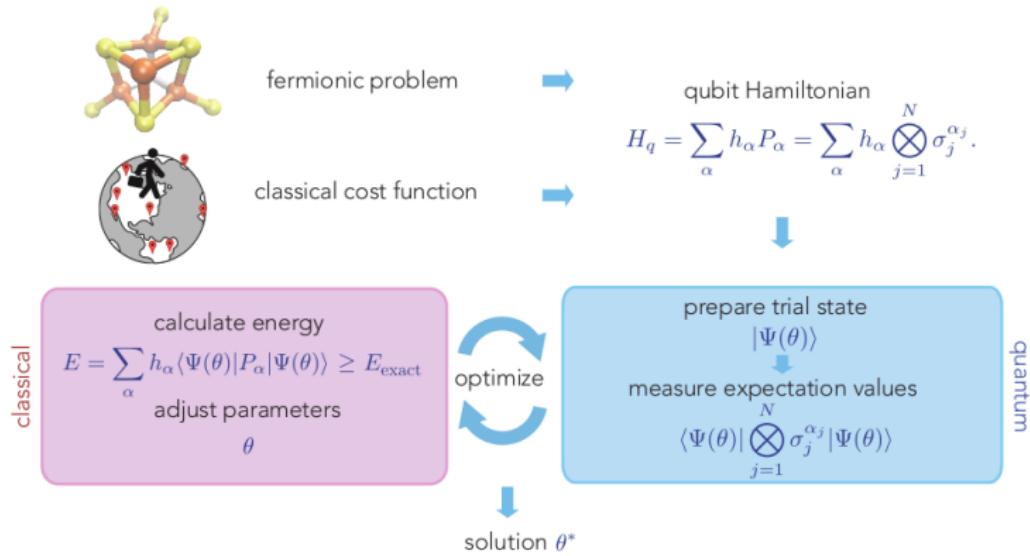
Figure: Scheme of a VQE procedure

[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.]

IBM

IBM has it's own quantum device, making available 14 real qubits for everyone who wants to try them.

It is also possible to use a quantum simulator with 32 qubits.

A 50 real qubits quantum computer will be available soon.
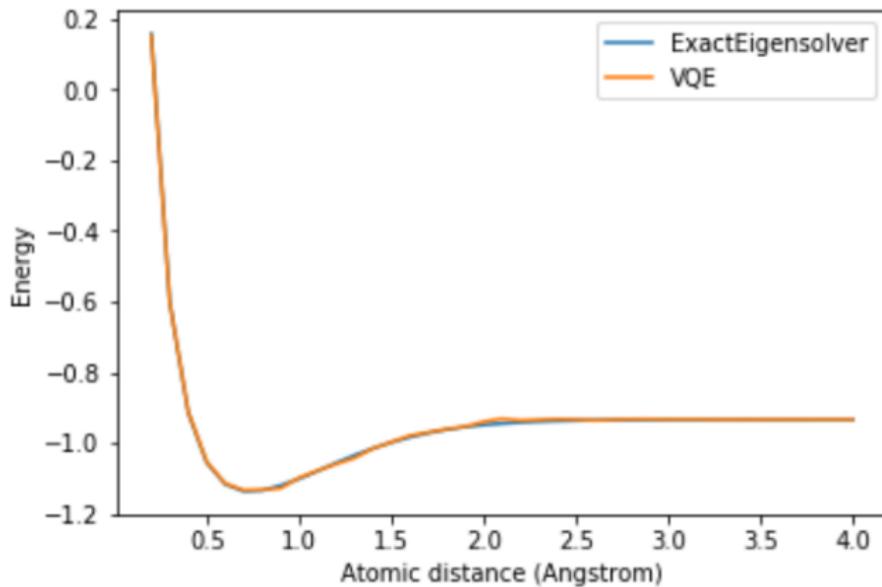
Results - H$_2$ molecule

Ground State Energies				
			ExactEigensolver	
			-1,137306035753	
			VQE method	
max_trials	depth	shots	Value	Variation
1	1	1	-0,712503938173	4,2E-01
		2048	-0,102521694036	1,2E+00
	7	1	-0,313978701260	8,2E-01
		2048	-0,593980785118	5,4E-01
5000	1	1	-1,137262155450	4,4E-05
		2048	-1,137304046500	2,0E-06
	7	1	-1,137304559058	2,3E-06
		2048	-1,137304311791	1,7E-06

Figure: The ground state energy is the lowest where a physical system can be. The energy unit used is the *Hartree*, an atomic unit of energy. The variation is the absolute error between the values obtained through Exacteigensolver and VQE method.

Results - H$_2$ molecule

Figure: Variation of the H_2 dissociation energy as the distance between atoms increases; parameters used in the VQE method: max_trials=350, depth=3 and shots=2048.

Results - LiH molecule

Ground State Energies					
			ExactEigensolver		
			-7,88240193229		
			VQE method		
max_trials	depth	shots	Value	Variation
1	1	1	-7,021299390490	8,6E-01
		2048	-7,191895551060	6,9E-01
	7	1	-7,052667867887	8,3E-01
		2048	-6,973986243448	9,1E-01
5000	1	1	-7,862023833205	2,0E-02
		2048	-7,857451742601	2,5E-02
	7	1	-7,880613192926	1,8E-03
		2048	-7,879721385780	2,7E-03

Figure: The ground state energy is the lowest where a physical system can be. The energy unit used is the *Hartree*, an atomic unit of energy. The variation is the absolute error between the values obtained through Exacteigensolver and VQE method.

Expectations for the Future

So where do Quantum computation stands now?
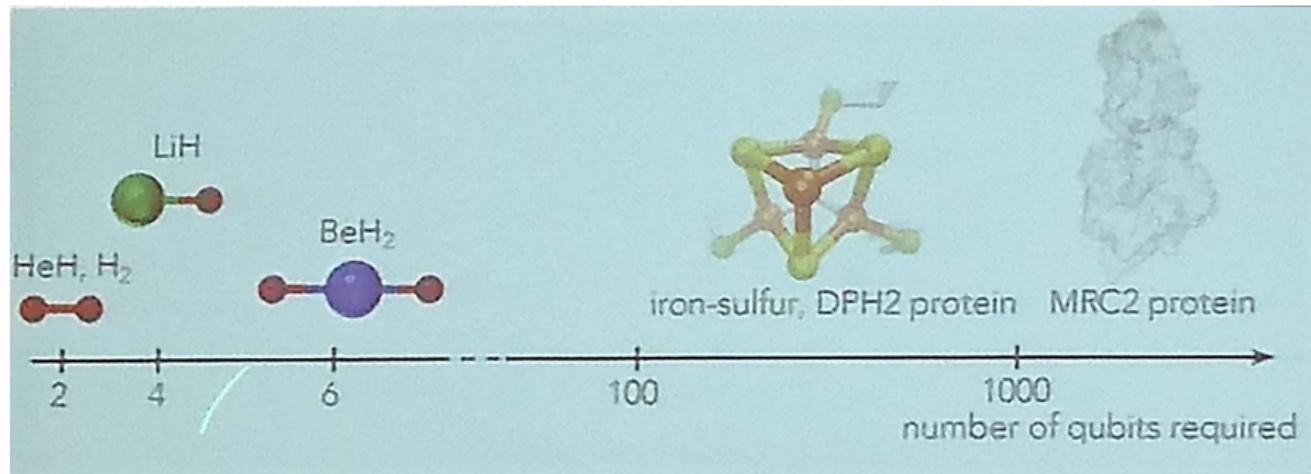
Figure: Number of Qubits per molecule - IBM Research

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.]

With more qubits great things are expected!