"A brief journey on quantum computation"

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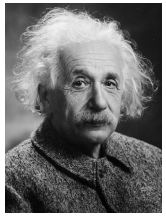
Overview

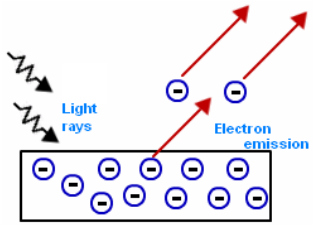
Quantum Theory

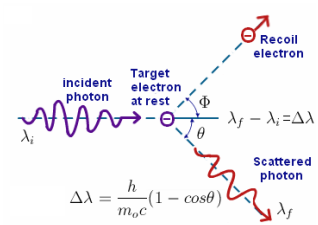
Old Quantum Theory

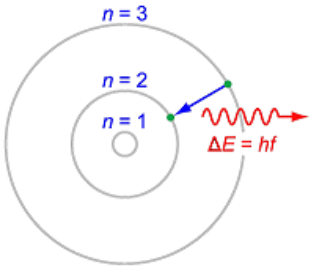
- In the beggining, there were only a set of radical ideas to solve several issues in classical physics
- Black-body radiation, Compton and Photoelectric effects, Atomic structure

$$u(\nu, T) = \frac{8\pi\hbar}{c^3} \frac{\nu^3}{e^{\hbar\nu/kT} - 1}$$









- It was then necessary to unify these ideas into coherent foundations and thus was born quantum mechanics.

Wave Formulation - Erwin Shrödinger

- Erwin Shrödinger formulated quantum physics as waves

$$\psi(x,t) = Ae^{i(kx-wt)} + Be^{-i(kx-wt)}; k = p/\hbar; \omega = E/\hbar \tag{1}$$

- Central of this formulation is the Shrödinger's equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\psi(x,t) \tag{2}$$

Wave Formulation - Erwin Shrödinger

There are several possible solutions in the Shrödinger equation... what does this mean?

Actually, a quantum system can be in several states (superposition) with probability given by $\Psi^*\Psi$ where * is the conjugate transpose of the wave (Born Interpretation).

Waves interfere!

The hydrogen atom

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

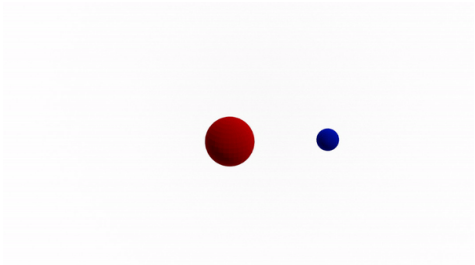


Figure: The hydrogren atom

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

$$\psi_{nlm}(r,\vartheta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)\frac{n-l-1!}{2n(n+l)!}}e^{-\frac{p}{2}}L_{n-l-1}^{2l+1}(p)Y_l^m(\vartheta,\varphi) \qquad (3)$$

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*]

Werner Heisenberg - Matrix mechanics

- Alternative formulation of quantum mechanics, states are represented by matrices.
- Observables (Hermitian operators) do not generally commute:

$$[A, B] \neq 0 \text{ for A and B observables and [A, B]} = \text{A.B - B.A}$$

- Most famous example: *Heisenberg uncertainty principle*: $[position, momentum] \neq 0$

The Hilbert space formulation I

Schrodinger's formulation happens in the space l_2, the space of all square summable complex sequences, and the Heisenberg's in the $L_2(\mathbb{R}^3)$ space,

Definition

A Hilbert space is a vector space H, over the complex numbers $\mathbb{C}$, with an internal product of type:

$$\langle -|- \rangle : H \times H \to \mathbb{C}\,. \tag{4}$$

Hilbert spaces of infinite dimensions must be Cauchy complete.

Dirac Notation

The Hilbert space formulation II

$|\Psi\rangle = \alpha_1 |\Psi_1\rangle \ldots + \alpha_n |\Psi_n\rangle$ where α_i are amplitudes and Ψ_i are elements of a basis of the vector space .

$$|\Psi\rangle = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{bmatrix} . \qquad \langle\Psi| = |\Psi^*\rangle^T = [\alpha_1^*, \alpha_2^*, \ldots, \alpha_n^*] .$$

$$\langle\Psi_1|\Psi_2\rangle = [\alpha_1^*, \alpha_2^*, \ldots, \alpha_n^*]. \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_3 \end{bmatrix} . \tag{5}$$

The Hilbert space formulation III

Postulate

The state space of an isolated physical system is the set of unitary vectors of an Hilbert space.

$$|\langle\Psi|\Psi\rangle|^2 = 1 \tag{6}$$

Postulate

The evolution of a quantum system is unitary: $U.U^\dagger = I$.

Postulate

The timed evolution of a quantum system is given by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle\,. \tag{7}$$

The Hilbert space formulation IV

Corollary

The evolution of a quantum closed system is equivalent to:

$$|\Psi_{t+\delta t}\rangle = e^{H\delta t} |\Psi_t\rangle \ , \tag{8}$$

Postulate

Measurements cause the collapse of quantum states into classical states. Mathematically, they correspond to projection operators: $|M_m\rangle \langle M_m|$, *where* m *is the desired outcome.*

The Hilbert space formulation V

Postulate

The state space of a composite physical system corresponds to the tensor product of the state spaces of the component physical systems. A tensor is operator

$$\otimes : \mathbb{C}_1^n \times \mathbb{C}_2^n \rightarrow \mathbb{C}^{n_1+n_2} \, . \tag{9}$$

Quantum mechanics

- Quantum mechanics is strange!
  - Interference!
- What is a measurement? What causes the collapse of the wave function?
  - Copenhagen interpretation
  - Multiverse interpretation

Quantum mechanics

Other strange factor: **entanglement**!

An important observable on particles: spin!

Spins in different axis do not commute $[\sigma_x, \sigma_z]! = 0$.

It is possible to build single states: states where total spin of two partices is 0.

$$|0_2\rangle \rightarrow |0_1\rangle \text{ and } |1_2\rangle \rightarrow |1_2\rangle$$

It is possible to build non-separable states!

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Quantum mechanics

Proposed by Einstein, Podolsky, Rose as a glitch in QM (EPR paradox)

- "Spooky action at a distance"

It has been demonstrated experimentally multiple times, by the demonstration of existence of correlations between the observations made in both particles!

One of the most important resources of quantum computation!

There has been intensive efforts to find mathematical tools to identify such states (quantum witnesses) and to quantify them!

Quantum computers depend on the ability to conserve resources, either interference and entanglement!

Quantum Computation

Quantum Computation

- Created in the eighties by Richard Feynman (Quantum simulation) and David Deutsch (Universal Quantum Computer);


- "Memory"
  - Qubit is the fundamental unit of information (as similarly to bit)

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,; |\alpha|^2 + |\beta|^2 = 1 \tag{10}$$

  $|0\rangle\,, |1\rangle$ are an orthogonal basis.
  - This can be extended to arbitrary dimensions, e.g. 2 dimensions

$$|\psi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + \lambda\,|11\rangle\,;$$

Quantum Computation

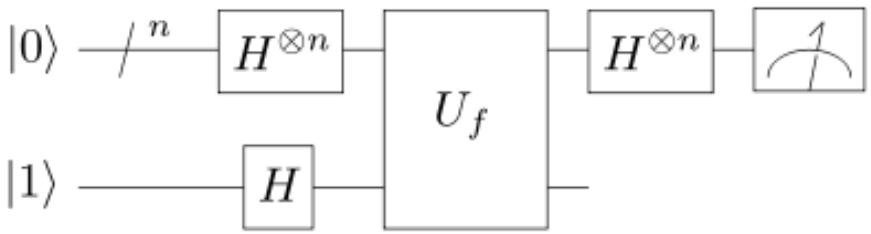
- Programs are
  - Linear unitary (reversible) operators of finite dimension ...

$$p : \mathbb{C}^{2^n} \rightarrow \mathbb{C}^{2^n} \tag{11}$$

  - ... or projection operators $|M\rangle \langle M|$.
- Consequences:
  - Only linear operators are possible, and hence, copies of states of variables are not possible (no cloning theorem).
  - Measurements destroy the status of the system (so as decoherence);
- Computer models:
  - Both models of Feynman (e^{iHt}) and Deutsch, so as perhaps any other quantum computing model fits these types.

Quantum Computation: the Circuit Model I

- Quantum circuit model:



- Quantum circuits are built out of sets of quantum gates.
- Any valid quantum transition operator can be approximated by circuits.

Quantum Computation: the Circuit Model II

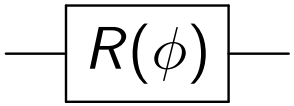
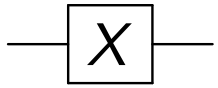
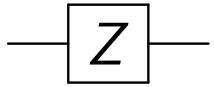
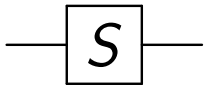
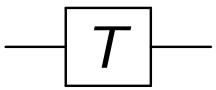
Gate	Circuit form	Matrix form
$R(\phi)$		$\begin{bmatrix} 1 & 0 \\ 0 & e^{-i\phi} \end{bmatrix}$
X		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
H		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
S		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{2}} \end{bmatrix}$
T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}$

Table: Single qubit gates.

Quantum Computation: the Circuit Model III

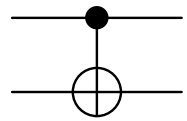
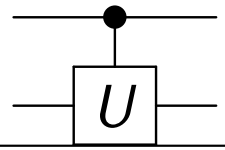
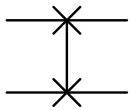
Gate	Circuit form	Matrix form
CNOT		$\begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix} \equiv \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
CU (Controlled unitary)		$\begin{bmatrix} I & 0 \\ 0 & U \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

Table: Two-qubit quantum gates.

Quantum computational complexity

Bounded Quantum Probability - contain *all* problems that are solvable in polynomial time by quantum computers-

- NP-Complete problems do not seem to be contained in BQP.
- Efficiency applies to all stages of the computation: from circuit generation to sampling.

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

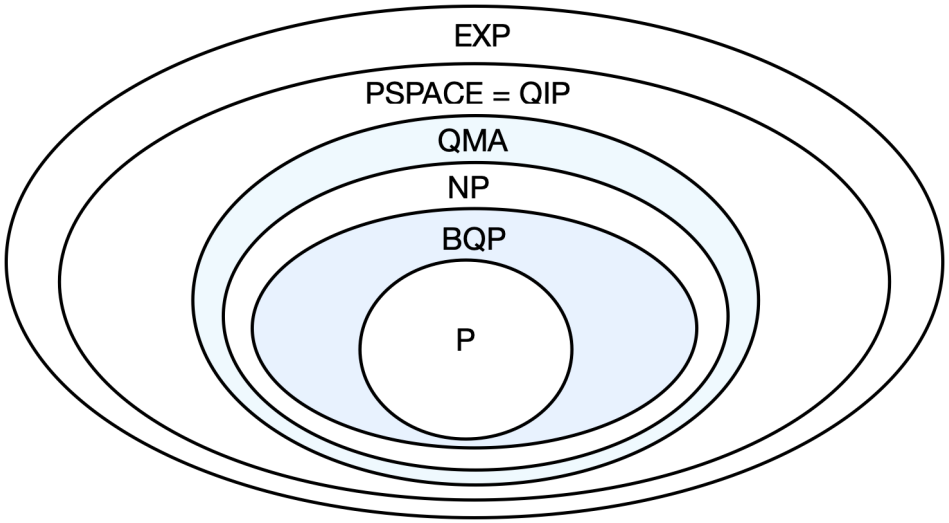
- Problems: QC-SAT, QC-Circuit, k-Local Hamiltonian, Density matrix consistency
- Finding the Ground State is hard even for a quantum computer, and in fact many classical optimization problems (NP-HARD) can be reduced to a ground state problem

Quantum computational complexity: exotic physics

Post BQP $\equiv$ **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 $\equiv$ **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.

Quantum Complexity classes



Logic and such

Semantics vs Complexity
Quantum advantage is clearly given in terms of resources, i.e. interference or entanglement, but resources do not seem to behave compositionally.

Expressibility Infinite dimensional quantum logic is undecidable, so as it seems the whole quantum theory at infinite dimensions. Hilbert are a third order language concept.

Efficient quantum algorithms

Deutsch-Jozsa Algorithm

- Created in 1992, by *David Deutsh* and *Richard Jozsa*.
- Verifies if a function of type $f : \{0, 1\} \rightarrow \{0, 1\}$ is *constant* or *balanced*.
  - Constant: $f(0) = f(1)$;
  - Balanced: $f(0) \neq f(1)$;
- It is the first algorithm that actually takes advantage of "quantum parallelism", working as a "proof of concept" of quantum advantage.

Deutsch-Jozsa Algorithm I

- The algorithm:
  - Prepare the system in the initial state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(\sum_{x=0}^{1}|x\rangle) \otimes (|0\rangle - |1\rangle)$$

  - Apply the oracle O over the state, evaluates both functions in a single step

$$O|\Psi\rangle = \frac{1}{\sqrt{2}}((-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle)$$

  - Example of an oracle for a function $f(0) = 0$ and $f(1) = 1$,

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

Deutsch-Jozsa Algorithm II

- Apply the Hadamard Gate and the final state will read as follows:

$$H|\Psi\rangle = \frac{1}{2}((-1)^{f(0)}(|0\rangle + |1\rangle) + (-1)^{f(1)}(|0\rangle - |1\rangle)$$

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

- The algorithm will always give $|0\rangle$ for constant functions, and $|1\rangle$ for balanced ones, i.e. the algorithm is **deterministic**. The algorithm is quite trivial, but generalizations do exist.

Shor algorithms

- Shor algorithm is the most relevant algorithm of quantum computation as it could potentially break RSA cryptography.
- Shor was inspired in Simon algorithm for the calculation of discrete logarithms.
- It is able to find the period of a periodic function $f(x)$, i.e. finds the r such that

$$f(x) = f(x + r)$$

- Or ... finds the generator of the hidden subgroup of a function.

Shor algorithms

- Consider a function with a group structure:

$$f : G \to \mathbb{N}, \text{ with } G \text{ being a group under some operation.}$$

- Each element e of the group generates a subgroup denoted as $\langle e \rangle$.
- Elements of the group, acting on the subgroup yield partitions, $g \circ \langle e \rangle$ ($\circ$ is the group operation) the so-called *cosets*;
- The *Hidden subgroup problem*: *Assume that* $f(g)$ *is constant on the cosets find* e.

- A periodic function is a $f : G \rightarrow \mathbb{N}$ where G is an Abelian group, under the $+$ operation:

x	0	1	2	3	4	5	6	7	8	9
f (x)	0	1	2	0	1	2	0	1	2	0

- The cosets are given as:

$$\{\{0, 3, 6, 9, ...\}, \{1, 4, 7, 10, ...\}, \{2, 5, 8, 11, ...\}\}$$

- And the subgroup that originates such cosets is $\{0, 3, 6, 9, ...\}$ and the generator is 3.

Shor algorithms I

- The algorithm
  - System preparedness

$$|\Phi\rangle = \frac{1}{2^{n/2}} \left(\sum_{x=0}^{2^n-1} |x\rangle \right) \otimes |0 \ldots 0\rangle \tag{12}$$

  - Entangle $f(x)$ in co-domain register with the correspondent x in the domain register

$$|\Psi_f\rangle = U_f |\Phi\rangle = \frac{1}{2^{n/2}} \left(\sum_{x=0}^{2^n-1} |x \otimes f(x)\rangle \right) \tag{13}$$

  - O estado do sistema pode então ser reescrito da seguinte maneira:

$$|\Psi\rangle = \frac{1}{\sqrt{2^n/K}} \sum_{i=0}^{2^n/K-1} \frac{1}{\sqrt{K}} \sum_{k=0}^{K-1} |x_i + kr\rangle |f(x_i)\rangle \tag{14}$$

Shor algorithms II

- Measure the counter domain register such that the coset will be identified.

$$|\Psi_0\rangle = \frac{1}{\sqrt{K}} \sum_{k=0}^{K-1} |x_0 + kr\rangle \tag{15}$$

- Then apply the Fourier transform over the domain register.

$$\frac{1}{2^{n/2}} \frac{1}{\sqrt{K}} \sum_{k=0}^{K-1} e^{2i\pi y(x_0+kr)/2^n} |y\rangle \tag{16}$$

- The probability is given

$$p(y) = \frac{1}{2^n} \frac{1}{\sqrt{K}} \left| \sum_{k=0}^{K-1} e^{2i\pi kyr/2^n} \right|^2 \tag{17}$$

- r can be extracted efficiently from this state: Fourier sampling.

Groups and Fourier Transform

- The quantum algorithm for the Hidden subgroup problem (which includes Shor) yields an exponential advantage to the classical ones:
- The advantage is the Fourier transform
  - Classic: $NlogN$, Quantum: $(log_2 N)log(log_2 N)$
- Fourier sampling has other possible applications: *Phase estimation*, *Eigenvalue estimation*, *Resolution of linear equations*.

Groups and Fourier Transform

- The same cannot be done with non-Abelian groups (operation is not commutative). The fourier transform in this groups does not provide an orthogonal basis, preventing the existence of efficient sampling algorithms.
  - Dihedral group (Lattice based cryptography) and the group isomorphism problem.
- Other applications? Spectral analysis on complex data?

Quantum simulation

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.]

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:

$$\left|\tilde{\psi_0}\right\rangle \leftarrow |\psi_0\rangle$$
$$j = 0$$
$$while(t_i + j * \Delta t < t_f)$$
$$\left|\tilde{\psi_{j+1}}\right\rangle = U_{\Delta t} \left|\tilde{\psi_j}\right\rangle$$
$$|\psi(t_f)\rangle = \left|\tilde{\psi_j}\right\rangle$$

Approximating $U_{\Delta t}$

A wide class of Hamiltonians can be approximated in this way [1], e.g. local Hamiltonians which possess components acting in subspaces of at-most dimension k

$$H = \sum_{i=1}^{m} H_i^k, \text{ where k is the dimension of the component}$$

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

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

[1] [Seth Lloyd. Universal quantum simulators. Science, pages 1073–1078, 1996.]

Approximating $U_{\Delta t}$

Evolution of a quantum system:

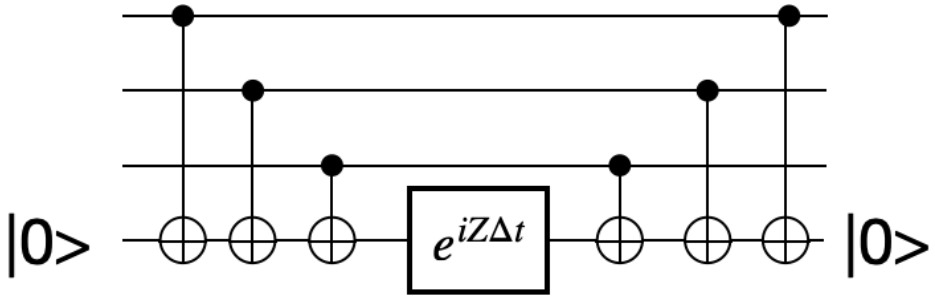
$$|\Psi_n(t)\rangle = e^{\frac{iE_n t}{\hbar}} |\Psi_n(0)\rangle \tag{18}$$

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

$$H_S = T^\dagger H_{S-diag} T \tag{19}$$

The correspondent evolutions reads as follows:

$$e^{-iH_S t} = T^\dagger e^{-iH_{S-diag} t} T \tag{20}$$

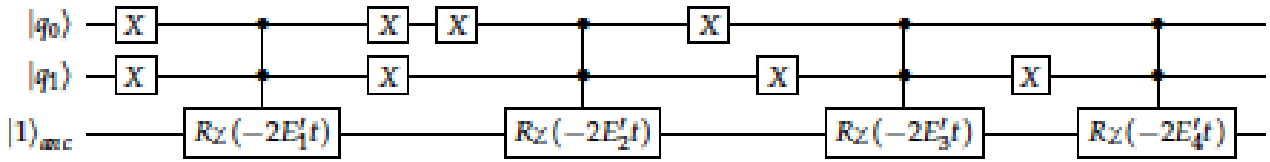
However T, $T^\dagger$ may be hard to calculate

Diagonal Hamiltonians

Considering a diagonal Hamiltonian:

$$\begin{pmatrix} e^{-iE_1 t} & 0 & 0 & 0 \\ 0 & e^{-iE_2 t} & 0 & 0 \\ 0 & 0 & e^{-iE_3 t} & 0 \\ 0 & 0 & 0 & e^{-iE_4 t} \end{pmatrix} \tag{21}$$

A possible circuit to this Hamiltonian reads as follows:



Simulation of the Schrödinger's equation

Schrödinger's equation:

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

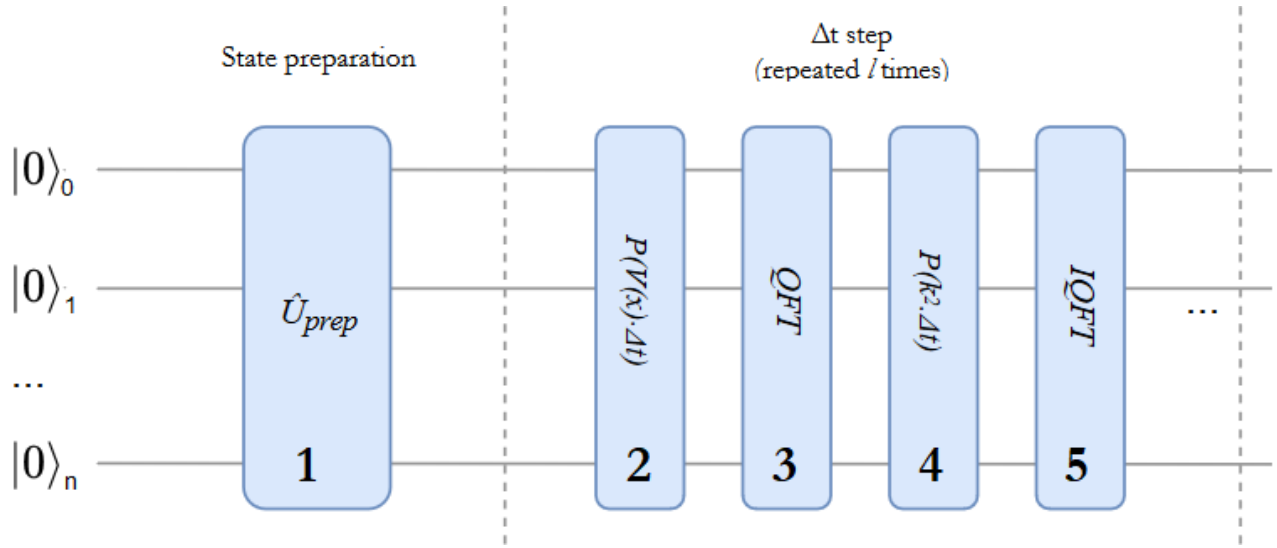
Iterative evolution of Schrödinger's equation:

$$\psi(x_i, t + \Delta t) = e^{-ik^2\Delta t}e^{-iV(x_i)\Delta t}\psi(x_i, t) \tag{22}$$

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.

$$F^{-1}e^{-ik^2\Delta t}Fe^{-iV(x_i)\Delta t} \tag{23}$$

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:

$$\lim_{x\to\infty}(e^{iAt/n}e^{iBt/n})^n = e^{i(A+B)t} \tag{24}$$

$(e^{iAt/n}e^{iBt/n})^n + \epsilon = e^{i(A+B)t}$, where $\epsilon = \mathcal{O}(\Delta t^2/N)$ and n sufficiently large (25)

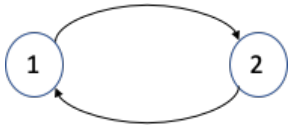
Baker-Campbell-Hausdorff Formula:

$$e^{i(A+B)\Delta t} = e^{iA\Delta t}e^{iB\Delta t}e^{-\frac{1}{2}[A,B]\Delta t^2} + O(\Delta t^3) \tag{26}$$

Algorithm I

Qubit encoding

Chain of molecules modelled in **site basis:** $\text{mol}_1 \mapsto |0\rangle, \text{mol}_2 \mapsto |1\rangle, \ldots$.
An example of chain can be modelled as a graph,



and the transport of energy would correspond to the transition of the state 1 to 2, i.e. $|0\rangle$ to the state $|1\rangle$.

Hamiltonian

$$\hat{H}_S = \sum_{m=0}^{N-1} \epsilon_m |m\rangle \langle m| + \sum_{m \neq n} J_{mn} |m\rangle \langle n| \equiv \hat{H}_S = \begin{pmatrix} \epsilon_0 & J \\ J & \epsilon_1 \end{pmatrix}$$

Algorithm II

Hamiltonian plus environment

$$\hat{H} = \hat{H}_S + \hat{H}_F$$

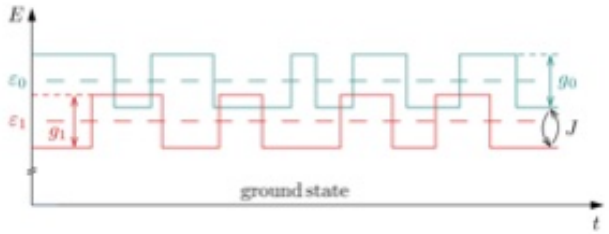
where

$$\hat{H}_F = \sum_{m=0}^{1} \chi_m(t)\hat{A}_m$$

and $\hat{A}_m |m\rangle \langle m|$ is the projection operator and χ_m is one fluctuator interacting with each molecule m,

$$\chi_m(t) = g_m \xi_m(t)$$

$\xi_m(t)$:

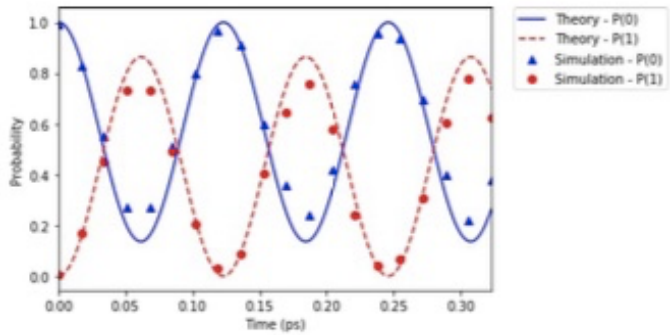


Experiments

Near-resonant regime

- $|E_1 - E_0| << J$

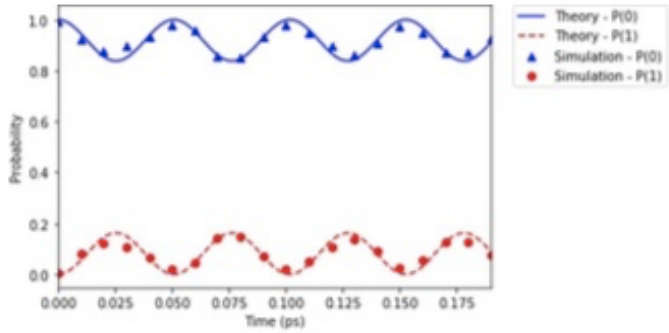
$$H_S = \begin{pmatrix} 13000 & 126 \\ 126 & 12900 \end{pmatrix} cm^{-1}$$



Non-resonant regime

- $|E_1 - E_0| >> J$

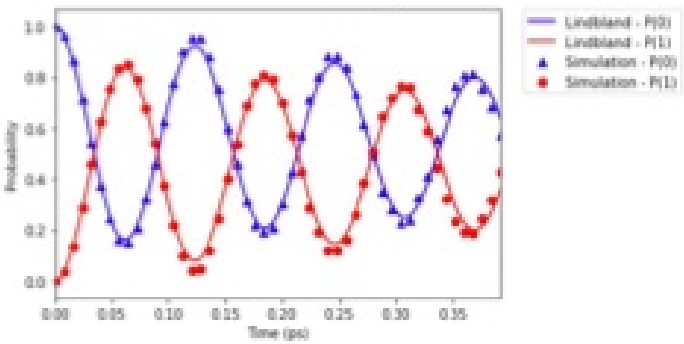
$$H_S = \begin{pmatrix} 12900 & 132 \\ 132 & 12300 \end{pmatrix} cm^{-1}$$



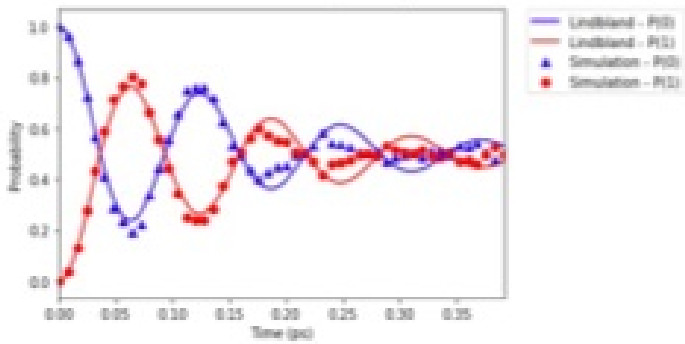
Experiments

Resonant Regime + Environment

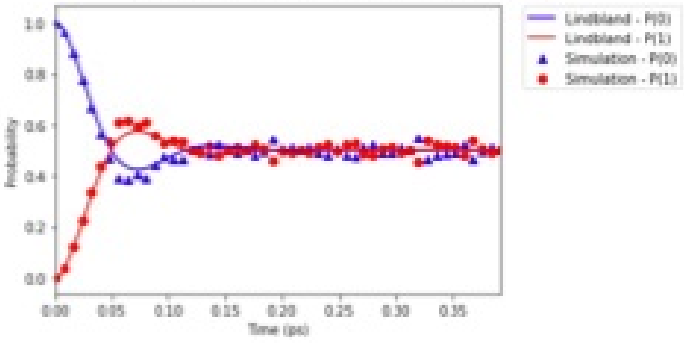
(a) $g = 100\ cm^{-1}$, $\gamma_{deph} = 2.3\ THz$.



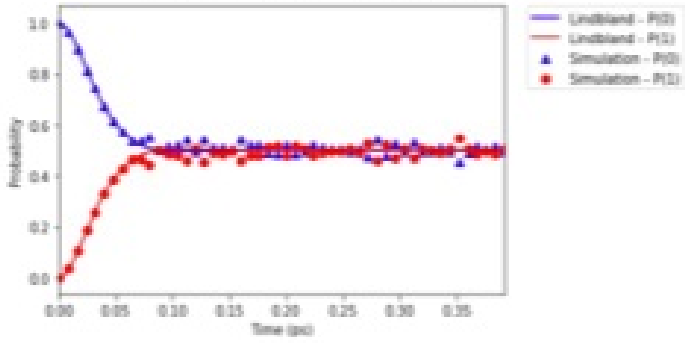
(b) $g = 300\ cm^{-1}$, $\gamma_{deph} = 10\ THz$.



(c) $g = 700\ cm^{-1}$, $\gamma_{deph} = 41\ THz$.

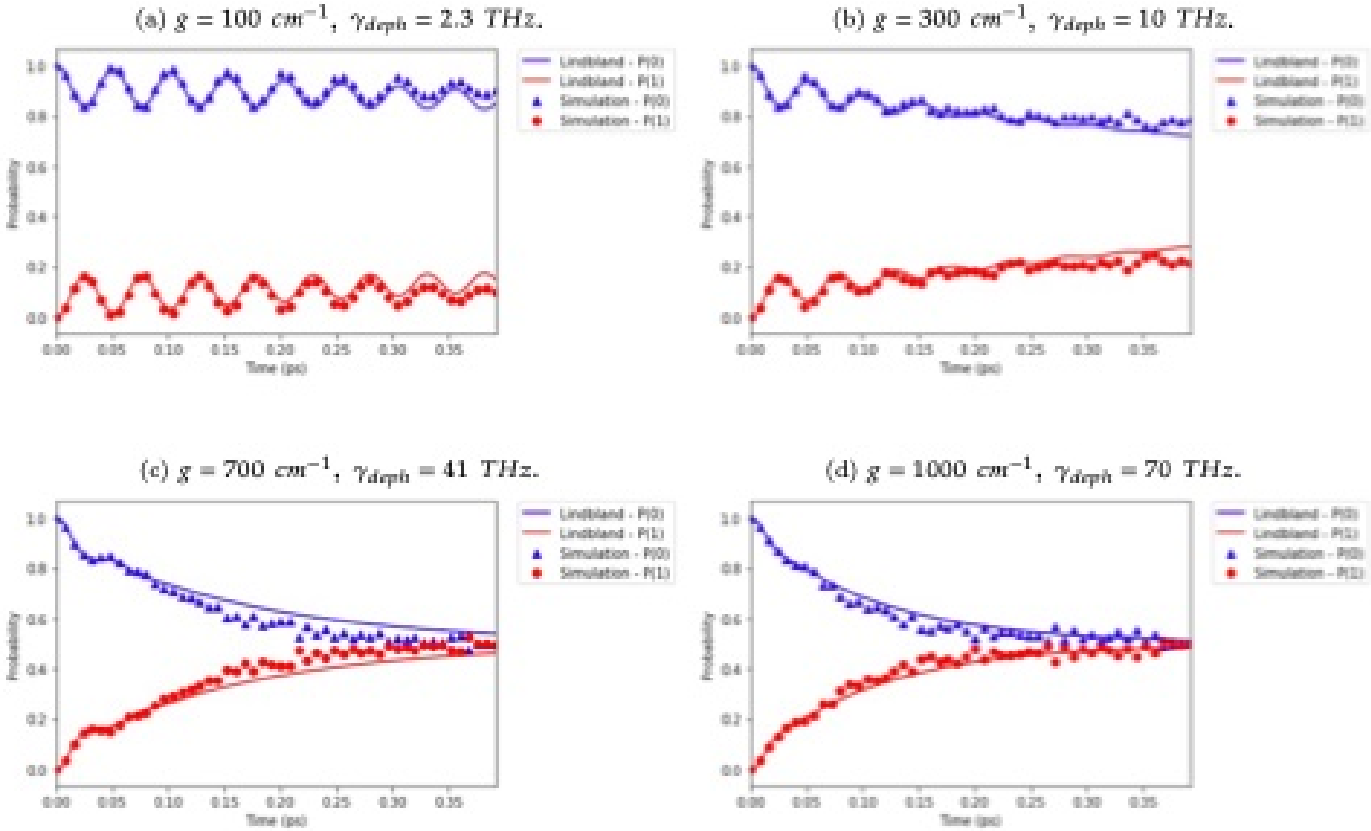


(d) $g = 1000\ cm^{-1}$, $\gamma_{deph} = 70\ THz$.



Experiments

Non-resonant regime + Environment



GUIMARÃES, José Diogo, et al. Simulation of nonradiative energy transfer in photosynthetic systems using a quantum computer. Complexity, 2020, 2020.

Applications of Quantum Algorithms

Combining Fourier sampling + quantum simulation brings yet another set of efficient quantum algorithms: HHL for solving linear equations which possesses a lot of applications including in machine learning[1].

[1] Duan, Bojia, et al. "A survey on HHL algorithm: From theory to application in quantum machine learning." Physics Letters A 384.24 (2020): 126595.

Industrial quantum algorithms

Optimization problems in quantum mechanics

Finding the ground state is an optimization problem:

$$\text{find } |\Psi\rangle \text{ that minimizes } H|\Psi\rangle$$

where H is an Hamiltonian, and Ψ can be

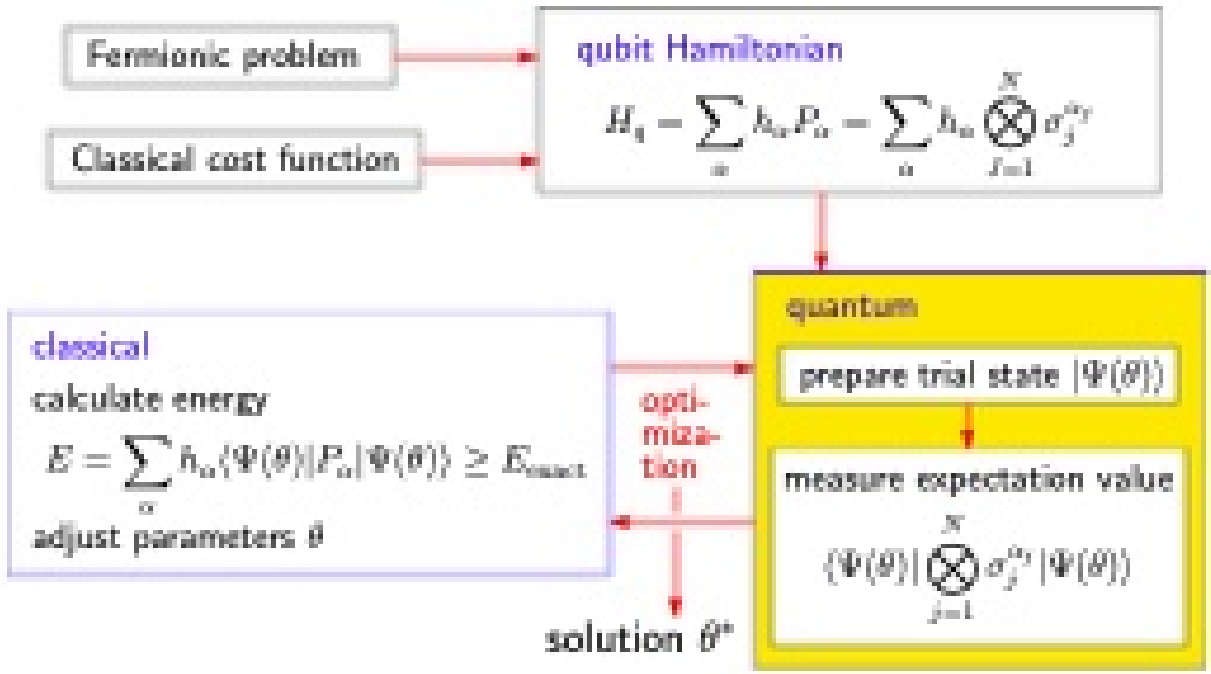
- $|\Psi\rangle = |\{0,1\}^n\rangle$, i.e. a definite state;
- $|\Psi\rangle = \alpha|\Psi_1\rangle + \beta|\Psi_2\rangle$, i.e. a superposition of states.
- It can become very complex very quickly:
  - Even with local Hamiltonians of dimension $d \geq 2$ are QMA-complete!

Optimization problems in quantum mechanics

- Quantum simulation vs finding the ground state
  - Simulation concerns the approximation the probability distribution of the evolution of an Hamiltonian, the ground state concerns its state of minimal energy.
- Other very well known quantum computational techniques such as the Grover algorithm can also be reduced to Ground-state problems.
- A wide class of optimization problems, such as binary optimization problems, can be reduced to ground-state problems, i.e. the ground state of the Ising Hamiltonian.

Techniques for solving ground-state problems

Several quantum algorithms to determine the ground-state of a quantum system: Adiabatic quantum computing, Iterative Grover algorithm, Iterative phase estimation;
The one that will be explored here: **Quantum variational methods**.



Figure

The variational Quantum Eigensolver

Hybrid (classical + quantum) optimization method consisting of classically determine the set of parameters $\vec{\theta}$ of a set of trial functions $\left|\Psi(\vec{\theta})\right\rangle$, that minimize the function

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

where the expected value of the Hamiltonian over such functions

$$\langle\Psi(\overrightarrow{\theta})|H|\Psi(\overrightarrow{\theta})\rangle$$

is evaluated by a quantum computer.

Quantum Expected value Estimation (QEE)

Calculation of the expected value of the Hamiltonian

$$\langle\Psi|H|\Psi\rangle = \sum_{i;\,q} h_q^i \left\langle \sigma_i^{(q)} \middle| \sigma_i^{(q)} \right\rangle + \underbrace{\sum_{\substack{i_1,i_2;\\ q_1,q_2}} h_{q_1,q_2}^{i_1,i_2} \left\langle \sigma_{i_1}^{(q_1)} \otimes \sigma_{i_2}^{(q_2)} \middle| \sigma_{i_1}^{(q_1)} \otimes \sigma_{i_2}^{(q_2)} \right\rangle + \cdots}_{M \text{ terms.}} \tag{27}$$

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	$O(M)$	$O(1)$	$O(\lvert h_{max}\rvert^2 M p^{-2})$
QPE	$O(1)$	$O(p^{-1})$	$O(p^{-1})$

The VQE method

The method involves:

- The definition of the Hamiltonian at hand and the calculation of all of the matrix elements;
- Its approximation using circuits in the computational basis;
- The appropriate choice of wave functions;
- The choice of ansatz;
- The calculation of the initial solution;
- The choice of classical optimization method.

Quantum chemistry

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.]

Quantum chemistry

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. 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

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

Stark effect Hamiltonian

The Stark effect consists of the study of the energy spectra of quantum systems under the action of a strong electrical field.

I start by a Fermionic Hamiltonian (Born-Oppenheimer approximation) and add the action of a static electric field

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

Second Quantization

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

$$\Psi(\chi_1, \chi_2) = -\Psi(\chi_2, \chi_1) \tag{28}$$

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)

$$a_i^\dagger \left|\chi_1\chi_2\ldots\chi_n\right\rangle = \left|\chi_i\chi_1\chi_2\ldots\chi_n\right\rangle ; a_i \left|\chi_i\chi_1\chi_2\ldots\chi_n\right\rangle = \left|\chi_1\chi_2\ldots\chi_n\right\rangle \tag{29}$$

[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	$h_{pq}a_p^\dagger a_q + h_{qp}a_q^\dagger a_p$	$\frac{1}{2}\left(\bigotimes_{k=q+1}^{p-1}\sigma_k^z\right)\begin{pmatrix}\Re\{h_{pq}\}(\sigma_q^x\sigma_p^x+\sigma_q^y\sigma_p^y)\\ +\Im\{h_{pq}\}(\sigma_q^y\sigma_p^x-\sigma_q^x\sigma_p^y)\end{pmatrix}$
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	$h_{pqqr}a_p^\dagger a_q^\dagger a_q a_r + h_{rqqp}a_r^\dagger a_q^\dagger a_q a_p$	$\left(\bigotimes_{k=r+1}^{p-1}\sigma_k^z\right)\left[\begin{pmatrix}\Re\{h_{pqqr}\}(\sigma_r^x\sigma_p^x+\sigma_r^y\sigma_p^y)\\ +\Im\{h_{pqqr}\}(\sigma_r^y\sigma_p^x-\sigma_r^x\sigma_p^y)\end{pmatrix}-\sigma_q^z\begin{pmatrix}\Re\{h_{pqqr}\}(\sigma_r^x\sigma_p^x+\sigma_r^y\sigma_p^y)\\ +\Im\{h_{pqqr}\}(\sigma_r^y\sigma_p^x-\sigma_r^x\sigma_p^y)\end{pmatrix}\right]$
Double Excitation Operator	$h_{pqrs}a_p^\dagger a_q^\dagger a_r a_s + h_{srqp}a_s^\dagger a_r^\dagger a_q a_p$	$\left(\bigotimes_{k=s+1}^{r-1}\sigma_k^z\right)\left(\bigotimes_{k=q+1}^{p-1}\sigma_k^z\right)\begin{pmatrix}\frac{\Re\{h_{pqrs}\}}{8}\begin{pmatrix}\sigma_s^x\sigma_r^x\sigma_q^x\sigma_p^x-\sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^y+\sigma_s^x\sigma_r^y\sigma_q^x\sigma_p^y\\ +\sigma_s^y\sigma_r^x\sigma_q^x\sigma_p^y+\sigma_s^y\sigma_r^x\sigma_q^y\sigma_p^x-\sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^x\\ +\sigma_s^x\sigma_r^y\sigma_q^y\sigma_p^x+\sigma_s^y\sigma_r^y\sigma_q^y\sigma_p^y\end{pmatrix}\\ +\frac{\Im\{h_{pqrs}\}}{8}\begin{pmatrix}\sigma_s^y\sigma_r^x\sigma_q^x\sigma_p^x+\sigma_s^x\sigma_r^y\sigma_q^x\sigma_p^x-\sigma_s^x\sigma_r^x\sigma_q^y\sigma_p^x\\ -\sigma_s^x\sigma_r^y\sigma_q^y\sigma_p^y-\sigma_s^y\sigma_r^x\sigma_q^y\sigma_p^y+\sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^y\\ +\sigma_s^y\sigma_r^y\sigma_q^x\sigma_p^y+\sigma_s^y\sigma_r^y\sigma_q^y\sigma_p^x\end{pmatrix}\end{pmatrix}$

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.]

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.

$$|\Psi(\overrightarrow{\theta})\rangle = \hat{U}(\overrightarrow{\theta})|\Psi_0\rangle\,, \tag{30}$$

Example of an ansatz: the UCC

$$\left|\Psi(\overrightarrow{\theta})\right\rangle = e^{\hat{T}(\overrightarrow{\theta})-\hat{T}^{\dagger}(\overrightarrow{\theta})}\,|\Psi_0\rangle\ . \tag{31}$$

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,

$$\hat{T}_1(\overrightarrow{\theta}) = \sum_{\alpha,a} \theta_\alpha^a a_a^\dagger a_\alpha , \tag{32}$$

$$\hat{T}_2(\overrightarrow{\theta}) = \frac{1}{2} \sum_{\alpha,\beta;\, a,b} \theta_{\alpha\beta}^{ab} a_a^\dagger a_b^\dagger a_\alpha a_\beta , \tag{33}$$

$$\dots$$

The actual optimization process

- Hartree-Fock approximation (Initial educated guess)

$$|\Psi_0\rangle$$

- Ansatz choice: *UCC Ansatz*

$$\left|\Psi(\vec{\theta})\right\rangle = e^{\hat{T}_1(\vec{\theta}) - \hat{T}_2(\vec{\theta})} |\Psi_0\rangle$$

where

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

$$\hat{T}_2(\vec{\theta}) = \sum_{a,\alpha,b,\beta} \theta_{\alpha\beta}^{ab} a_a^\dagger a_b^\dagger a_\alpha a_\beta$$

- Evaluate the expected value $E[\Psi(\vec{\theta})]$
- Generate new solution, i.e. by refinining $\vec{\theta}$, following classical optimization method, e.g. SPSP or Cobyla.

Quantum Computation: where to go?

The strugle for reliability qubits goes on:

- Qubit architectures: superconducting qubits, topological, ion traps, photonic machines.

Also with alternative computer models

- Measurement based computing, VQE methods...

A relevant topic: error mitigation techniques

- Random circuit generation, Zero-knowledge extrapolation[1]

[1] GUIMARÃES, José D.; TAVARES, Carlos. Towards a layered architecture for error mitigation in quantum computation. In: 2022 IEEE International Conference on Quantum Software (QSW). IEEE, 2022. p. 41-51.

Questions ?