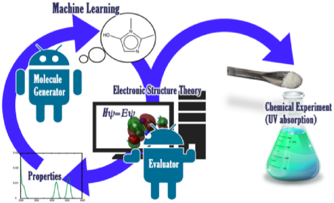
Variational Quantum Eigensolver

Marten Teitsma

January 15, 2024

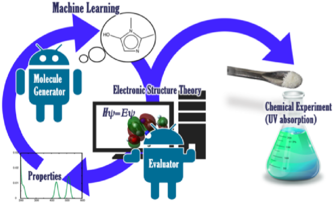
Contents

Computational Chemistry



- Branch of Chemistry using computer simulations to assist in solving chemical problems.
  - Understand the molecule with the aid of software
- What type of information do we get from it?
  - Structure (positions of the atoms)
  - Absolute and relative energies
  - Electronic charge density distribution

Computational Chemistry

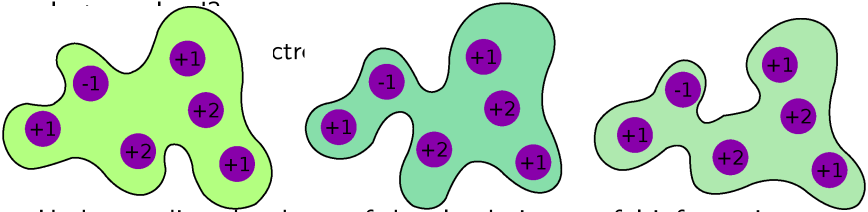


- Methods go from approximate to highly accurate
- Depend on what we are studying
  - Trial and error
  - Smart design of molecules
- Most accurate methods: Quantum Mechanics
- Ultimate goal:

  Finding the minimum energy state of a molecule

Problem

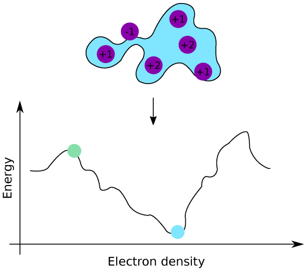
- Given a configuration of atomic nucleus, what is the shape of the

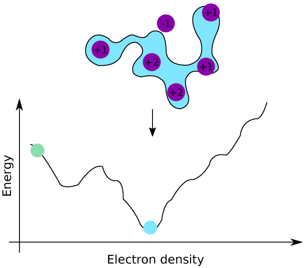


- Understanding the shape of the cloud gives useful information

Problem

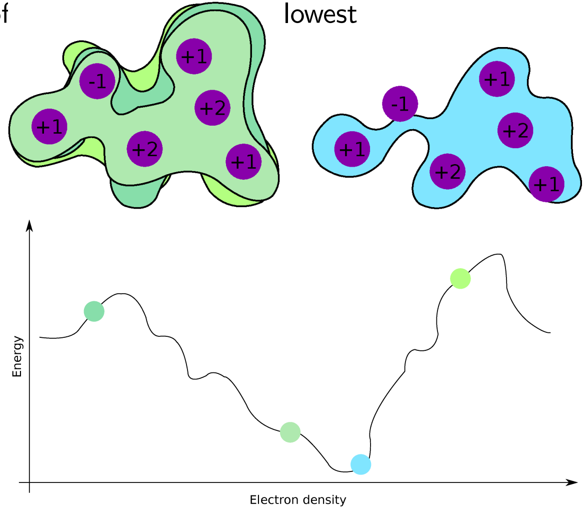
- Different configurations (molecules) lead to different energy landscapes and shapes of electronic clouds





Problem

- We want to find the “shape” of the electron cloud in which the energy of lowest



Problem

- Determine the lowest–energy state
- How to represent the energy of a system?
  - Hamiltonian operator $\hat{\mathcal{H}} = K + P$
  - Described by an Hermitian matrix
  - With real eigenvalues
- Use Schrödinger equation to obtain the energy:

$$\hat{\mathcal{H}} \left|\psi\right\rangle = E \left|\psi\right\rangle$$

- Expectation value for a quantum state:

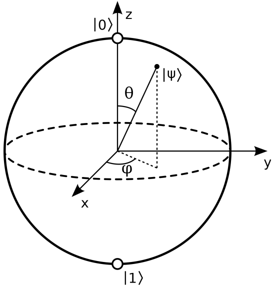
$$E_\lambda = \left\langle\psi_\lambda\right| \hat{\mathcal{H}} \left|\psi_\lambda\right\rangle$$

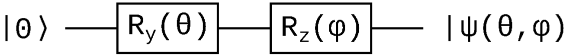
Problem

- Find the minimum eigenvalue of a matrix that represents its ground state energy
  - Ideally $\rightarrow$ exact minimum eigenvalue but ...
    - Fully coherent quantum computer
    - Quantum Phase Estimation algorithm
- $\Rightarrow$ Variational Quantum Eigensolver algorithm
  - Find the lowest eigenvalue associated with a given matrix
  - Close–to–perfect answers

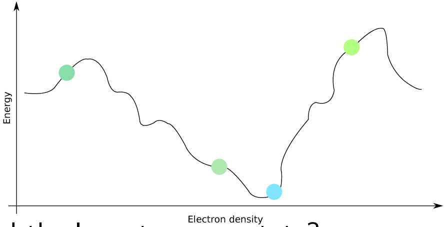
Variational solution

- Parameterized approach:
  - The state is described by some parameters



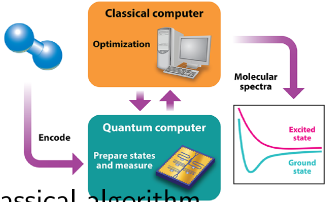


Variational solution



- How do we find the lowest energy state?
    1. Initial guess state
    2. Calculate the eigenvalue of the Hamiltonian
    3. Modify the parameters
    4. Calculate the eigenvalue. Has it improved?

Variational Quantum Eigensolver



- Hybrid quantum–classical algorithm
- Classical computer:
  - Measure and optimize the parameters
  - Iterate through the loop
- Quantum device:
  - Map the Hamiltonian: molecular $\rightarrow$ qubit
  - Prepare the ansatz
  - Calculate the energy

Variational Quantum Eigensolver

1. Mapping the molecular Hamiltonian into a qubit Hamiltonian

$$\hat{\mathcal{H}} = -\sum_i \frac{\nabla^2_{R_i}}{2M_i} - \sum_i \frac{\nabla^2_{r_i}}{2} - \sum_{i,j} \frac{Z_i}{|R_i - r_j|} + \\ + \sum_{i,j>i} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i,j>i} \frac{1}{|r_i - r_j|}$$

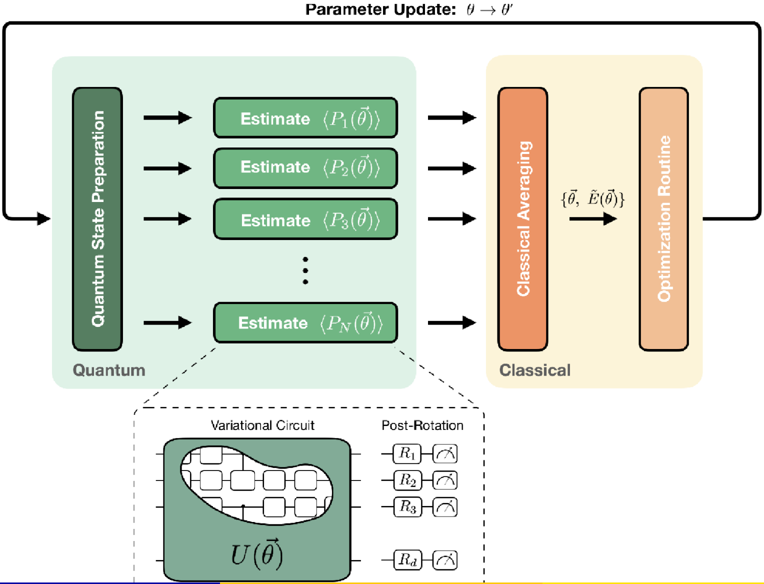
   - Use Jordan–Wigner or Bravyi–Kitaev transformations

2. Creating the trial state (ansatz)
   - Using a small set of parameters (θ)
   - Construct a parameterized trial guess $(\psi(\theta))$
   - Run it with the parameterized trial state

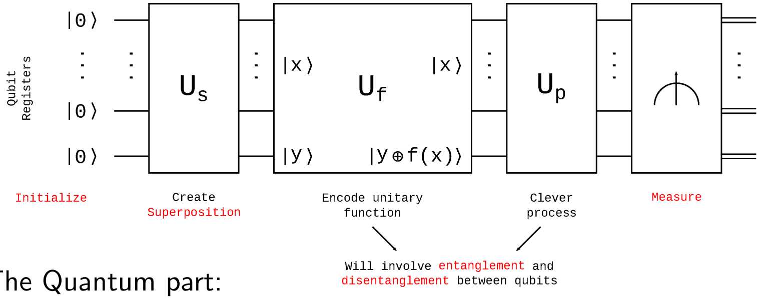
Variational Quantum Eigensolver

3. Calculating the energy
    - Measure the expectation values of the Hamiltonian
    - Calculate the energy of the trial state
4. Measure and optimizing the parameters
    - Optimization algorithm (e.g., gradient descent)
    - Update the parameters
5. Iterate through the loop
    - Until convergence

Variational Quantum Eigensolver



Variational Quantum Eigensolver



- The Quantum part:
  - Encode the molecular Hamiltonian into a quantum circuit
  - Prepare parameterized guess state
  - Measure the energy

What is next?

- Assignment is already available (check DLO)
- Q & A, Discussion
  - Questions about the assignment or the material
  - Feel free to propose any discussion
  - You can always write me an email