Orbitals - Speeding up Chemistry Simulations

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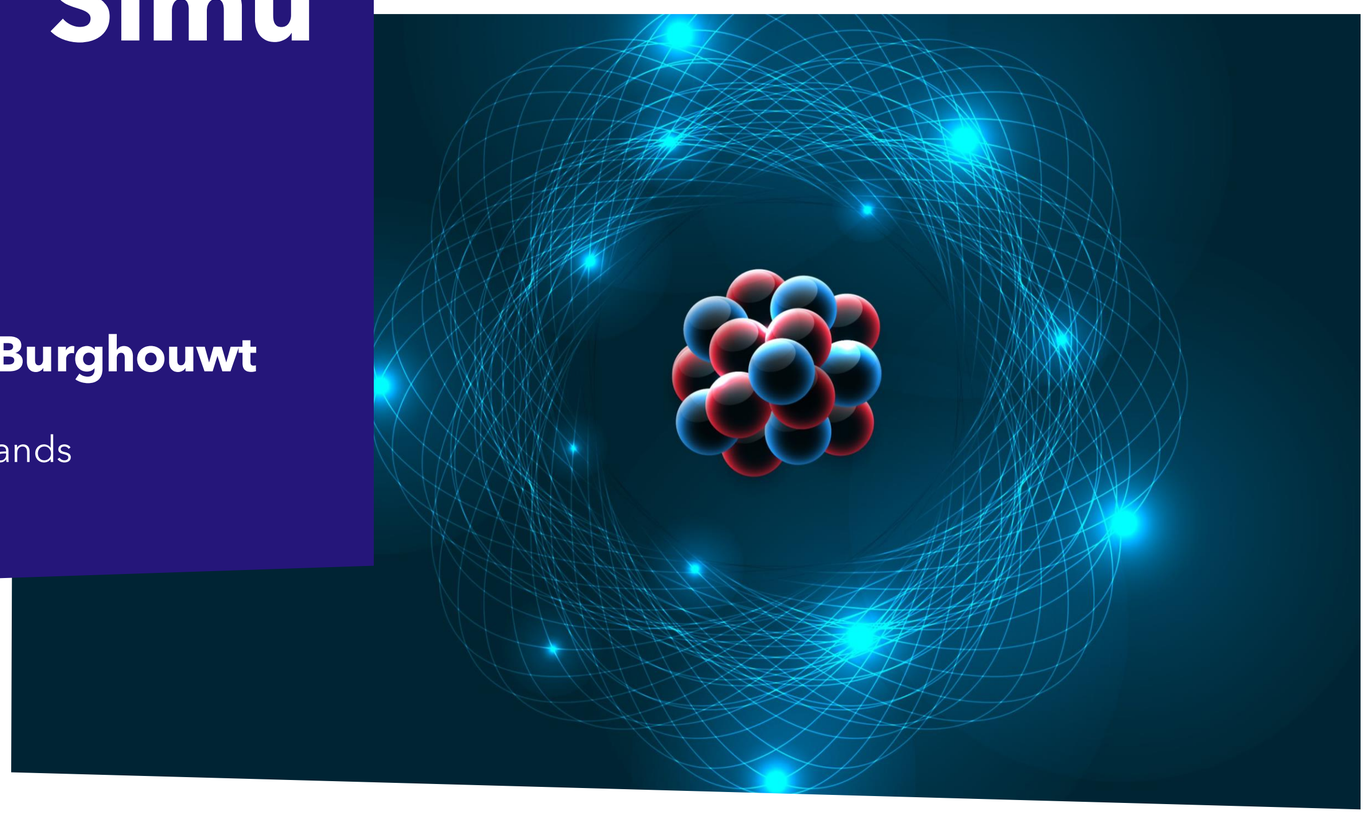


Introduction

In this project we use Quantum Simulation to calculate the ground and energy states of hydrogen molecules.

In our project we work on programs that:

- Use a simulated quantum computer to find the (ground) energy states of hydrogen molecules.
- Evaluates the simulation comparing 2 Quantum Software Development Kits (SDK's) in performance and accuracy.

Challenges

- **Using the SDK's to accurately calculate ground state energy levels and comparing performance.**
- **Implementing our programs on real quantum computers.**

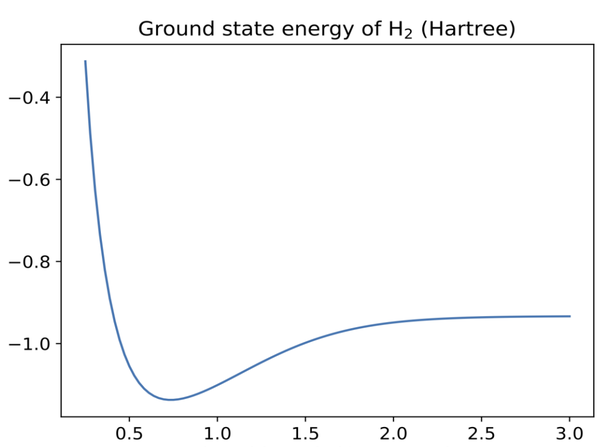
Methods

We will be using a Variational Quantum Eigensolver (VQE) to calculate the ground state energy levels.
Our method consists of two main parts:

- Finding the energy level of a molecule on a certain bond length (The VQE part).
- Using a classical search algorithm to find the ground state by looking for the lowest energy levels of the system at various bond lengths.

A VQE uses:

- A Hamiltonian: The definition of the state the system is in.
- An Ansatz: Describes how the quantum computer will find the ground state by creating a circuit that runs on the (simulated) quantum computer.



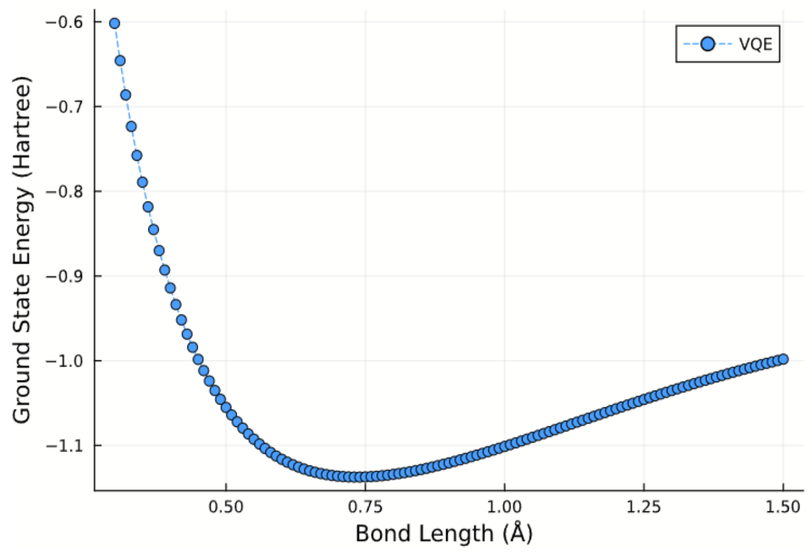
VQE: The energy of the system at various bond lengths: results in a curve.

Results

We used:

- IBM's Qiskit
- Yao: A quantum library for Julia (programming language).

We used the classical Golden-Section Search to find the minimum energy of the system.



The ground state energy levels at various bond lengths.

In the picture above we iterated through various bond lengths and calculated the ground energy state with an VQE.

Our results.
Interatomic Distance:

- Computed: 0.7348645578 Å

Ground Energy:

- Computed: -1.1373060512 Hartree

Largest Deviation from Exact Result:

- Distance: 6.0665321e-07 Å
- Energy: 5.7357896e-11 Hartree

Conclusion and next steps

- The results show that our programs can accurately find the ground state energy.
- The next step is to implement these programs on a real quantum computer.