Estimating ground state wavefunctions using **QPE** vs **VQE**

Quantum Phase Estimation vs. the Variational Quantum Eigensolver Method

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Introduction

In quantum mechanics, the **time evolution** of a quantum system is described by the Schrödinger equation[1]

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

where

- H denotes the **Hamiltonian** of the system.
- $\hbar$ is the **Plancks constant**
- $|\psi\rangle$ is the **state vector**

[1] Sakurai and Napolitano, *Modern Quantum Mechanics*.

Eigenvalue equation

Eigenvalue equation:

$$H|\psi\rangle = E|\psi\rangle$$

where E denotes the **energy** of the system.

The set of eigenstates $\{|\psi\rangle\}$, for which this equation holds, is of big importance in many fields.

Ground state

Of this set especially important is the **ground state**, i.e. the state $|\phi\rangle$ with the lowest observable energy E_0.

Classical intractability

The eigenvalue problem cannot efficiently be solved! Computational complexity of the Eigenvalue Problem for a $n \times n$ matrix:

$$O(n^p)$$

for some fixed p, depending on the algorithm.

Problem:

For a system of m qubits, the describing state vector $|\psi\rangle$ will have the size 2^m.

Thus the matrix description of H is $2^m \times 2^m$, resulting in complexity $O(2^{pm})$.

Quantum algorithms

However, the problem is often solvable efficiently on a quantum computer using dedicated algorithms.
Two of the most prominent examples are:

1. Quantum Phase Estimation (**QPE**)
   - Can be implemented purely on quantum registers
   - Provides high accuracy
   - More computationally expensive
2. Variational Quantum Eigensolver (**VQE**)
   - Quantum/ classical hybrid algorithm
   - Less accurate
   - Less computationally expensive

Quantum Phase Estimation (**QPE**)

- Starts with an **initial guess** of the ground state $|\psi'\rangle$
- Use auxiliary qubits in equal superposition to perform controlled operations on $|\psi'\rangle$
- Perform **inverse QFT** on them and measure results
- The measurement will cause the system to collapse into the true eigenstate $|\psi\rangle$

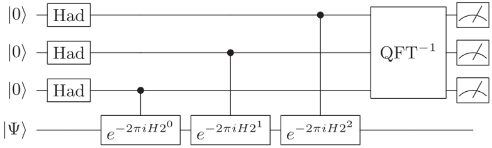

Figure 1: Circuit schema of the QPE algorithm [2]

[2] McArdle et al., "Quantum computational chemistry".

Variational Quantum Eigensolver (**VQE**)

- Use Parameterized **Ansatz** state (parameterized gates)
- Entangle Ansatz states
- **Optimize** over the measured energy by varying the gate parameters (e.g. gradient descent)
- The lowest possible energy corresponds to the **ground eigenstate**.

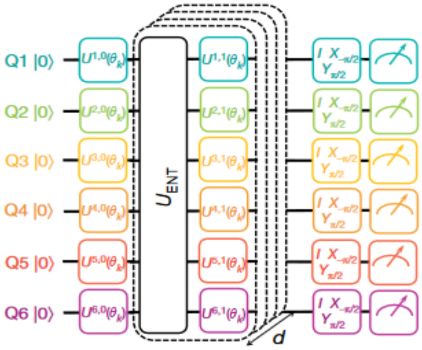

Figure 2: Circuit schema of the VQE algorithm [3]

[3] Kandala et al., "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets".

Thesis goals

- Create numerical implementations for QPE and VQE
- Solve the eigenvalue equation analytically for one or more example systems (atoms, molecules)
- Simulate the algorithms and the system on an existing quantum simulator (IBM, AQT, ...)
- Compare the results of the two algorithms
- Discuss the different advantages and disadvantages of the approaches

Time schedule

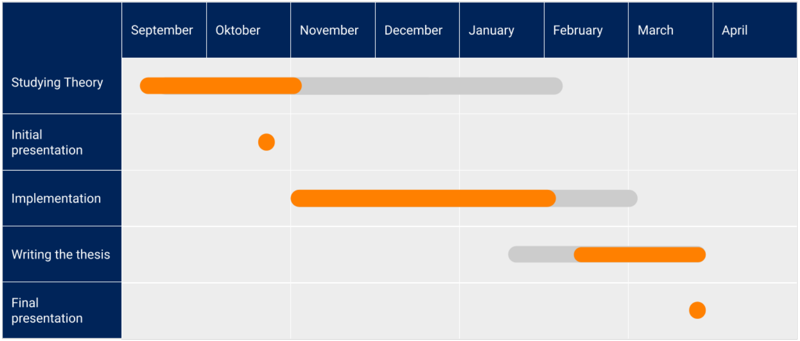

Figure 3: Time Schedule

Thank you for your attention!

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Appendix - Concrete molecules

Hardware restrictions

Due to the small amount of qubits available as of now, the molecules to have to be rather small.

Successful implementations have been done for molecules like Lithiumhydride LiH, or Berylliumhydride BeH_2.

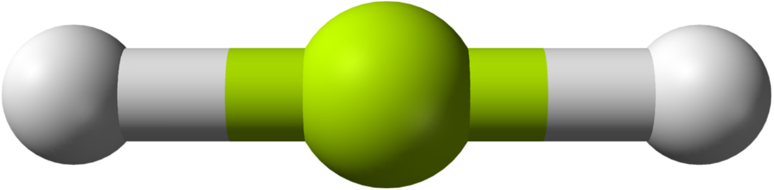

Figure 4: Berylliumhydride; **Creator:** Benjah-bmm27, Public domain, via Wikimedia Commons