Optimization Analysis on the Variational Quantum EigenSolver

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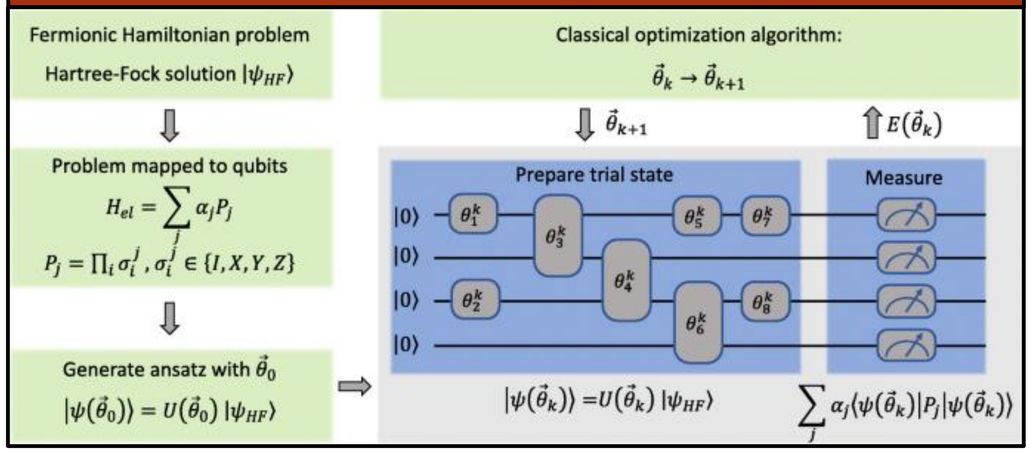
Overview

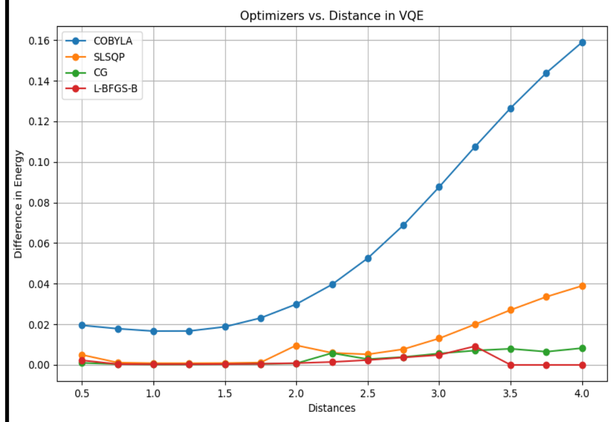
The Variational Quantum EigenSolver is a hybrid algorithm that uses both classical and quantum computers. It can solve optimization problems which in this project, it is used to find the minimum energy of a molecule. There are many type of optimizers and the algorithm iterates the results of the quantum circuit through the optimizer and back. Therefore, I conducted an optimization analysis on different optimizers and determined how many number of iterations are needed for maximum accuracy.

Algorithm Design



Research Results

COBYLA optimizer preformed the worse in terms of accuracy when simulating smaller molecules but each optimizer preformed the **same** when simulating bigger molecules.



Current Quantum computer could only simulate molecules up to 10 electrons, but the following data was collected to find how many iterations are needed through the optimizer for maximum accuracy.

Molecule	# Electrons	# Iterations
H2	2	4
LiH	4	8
BeH2	6	27
H2O	10	86

For more Information, check out my Github page https://github.com/Angelmartinez-20/Optimizer_Analysis_VQE . This include more research results, source code, and a research paper which was also submitted to the CSCSU 2024 conference and was accepted and published.

Initializing Problem

Classical computer constructs Hamiltonian Matrix which represents the total energy levels of a Molecule.

$$H = \hbar\omega \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & \dots \\ 0 & \frac{3}{2} & 0 & 0 & \dots \\ 0 & 0 & \frac{5}{2} & 0 & \dots \\ 0 & 0 & 0 & \frac{7}{2} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

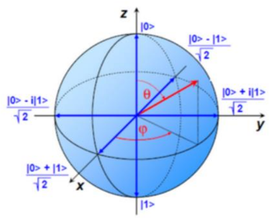
Hamiltonian matrix then gets broken down into smaller matrices which represent the Rotational Gates of the Quantum Circuit

Rotation matrices:

$$\hat{R}_x(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

$$\hat{R}_y(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

$$\hat{R}_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$



Ansatz is initialized by a classical algorithm such as the Hartree-Fock to set the initial parameter of the Quantum circuit which represent the trial wave function.

Classical Quantum Iteration

After the problem has been initialized into the quantum circuit, the quantum computer is able to apply entanglement through a series of CNOT gates which collectively explores parameter space. When the circuit is measured, the output is passed through an optimizer to update its parameters and iterates back to the quantum computer to find the global minimum energy of a molecule.

Tools

Qiskit

4-Qubit Quantum Circuit