



VQE Algorithm for Dihydrogen Ground State Energy

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Abstract

In this project, we implement the Variational Quantum Eigensolver (VQE) algorithm on our model for a dihydrogen (H_2) molecule. In our implementation, we create models for spin operators, projection operators, rotation operators, the basis vectors, and the Hamiltonian in matrix representation to calculate the ground state energy of dihydrogen at variable bond lengths. We compare our results for ground state energy with respect to current literature. We find the results to loosely mimic a generic potential curve. The lowest ground state energy calculated is very close to the accepted ground state energy of dihydrogen (~ 30 eV).

Research Goals

The goal of this project is twofold. First, we implement our own version of the VQE algorithm optimized for 2-qubit systems. With our implementation of the algorithm, we test how the ground state energy varies as a function of bond length. We focus on dihydrogen because it is the most common isotope of hydrogen found in nature and explore how the variational method operates in this system.

Our research question is as follows: How does the ground state energy change with bond length, as applied to the dihydrogen molecule, simulated using a VQE algorithm?

Background

The Variational Quantum Eigensolver (VQE) is an algorithm that combines methods of classical and quantum computation to estimate the ground state energies for different molecules. It has applications in quantum chemistry, condensed matter physics, and much more. Some simulations of the algorithm exist already, such as IBMQ's software, however for this project we implement our own using python. In our experiment, we focus on ground state energy as a function of intermolecular bond length.

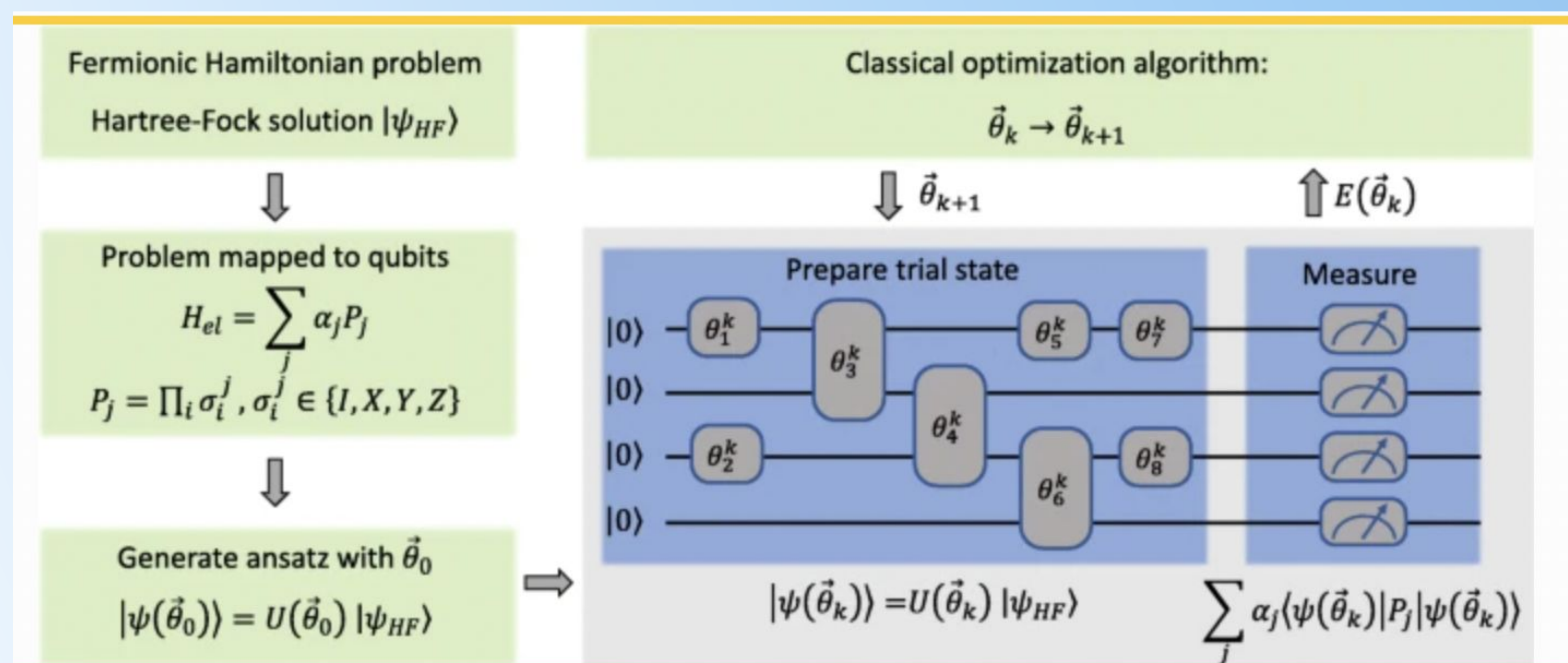
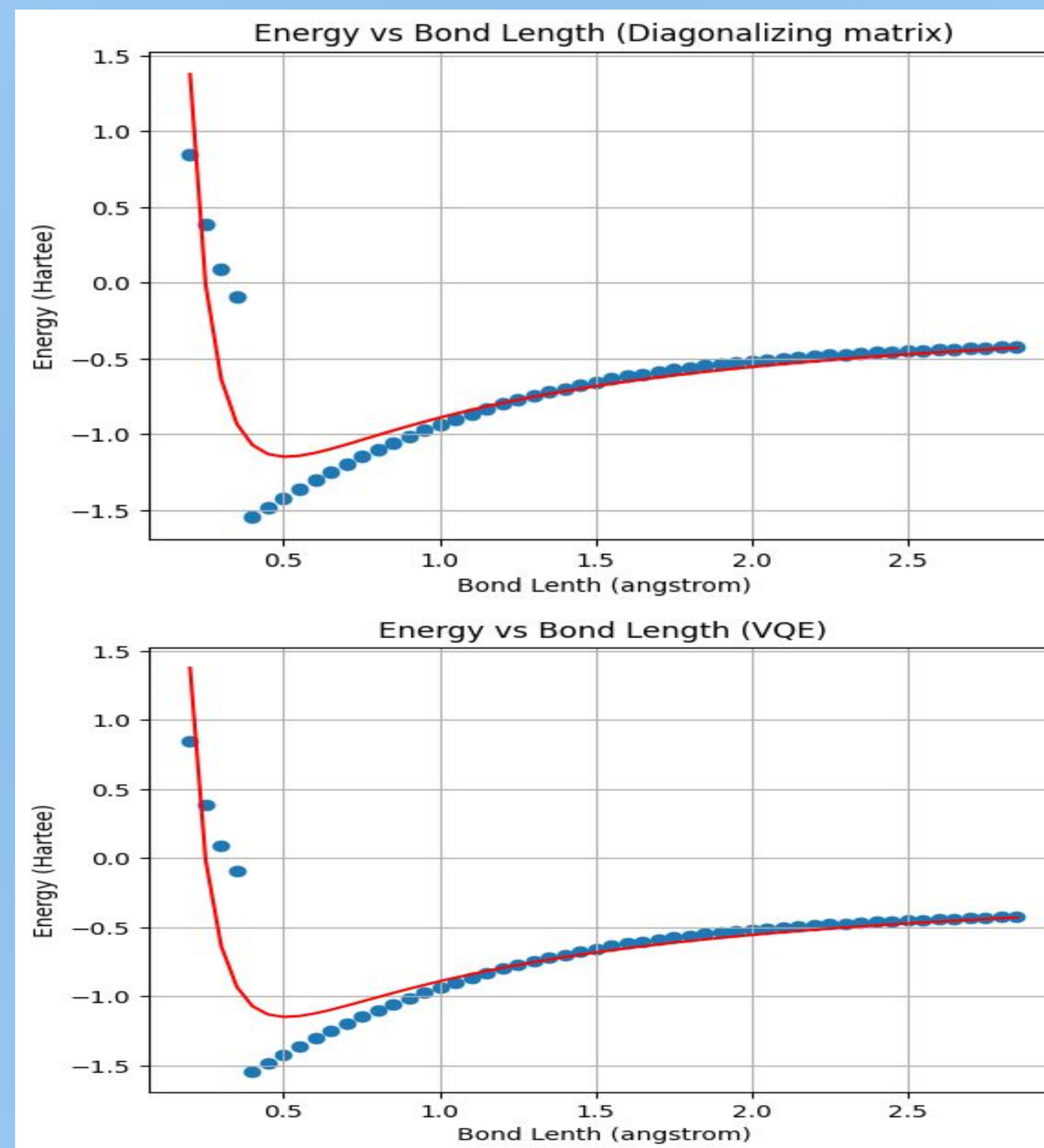


FIG 2. A roadmap of how the VQE algorithm works.

This bond length refers to the distance between an electron and the nucleus of the atom. Our algorithm can only afford hydrogen and helium, as we restrict our simulations to 2 qubit systems. More advanced VQE algorithms can handle systems with many more qubits. For this project, we focus on dihydrogen which is a covalent bond between two hydrogen atoms; this entails two electrons and two protons in total. The basis of his simulation rests on the Hartree-Fock theory, which describes the wave function of electrons as independent of one another. Hence, we approximate the electrons as not interacting with one another initially, and then proceed to consider interactions.

Results

This is the graphic representation of our data as energy in Hartrees over bond length in Angstroms. The first graph depicts the results of applying the quantum operators directly (diagonalizing the Hamiltonian), while the second shows our tabulated results from running our algorithm. Therefore, the results of our algorithm match what we should expect, and the two are in almost perfect agreement (which is a good indication of accuracy). However, our model does not account for the change in scaling at the local minimum around ~ 0.5 Angstroms, which led to substantial error as our model continued towards zero.



Conclusion

Let's first discuss the strengths of our results. The lowest calculated ground state energy that we receive from our algorithm is ~ -1.17 Hartrees = -31.83732 eV, whereas O'Malley et al's paper calculates the lowest ground state energy as -1.15 Hartrees = -31.83732 eV¹. Thus, while our result is not exact, we have achieved an impressively accurate result with respect to literature.

As a function of intermolecular bond length, the calculated results for ground state energy do not match the shape of the generic potential curve we should expect. This is because the scaling of the ground state energy with respect to bond length changes at the local minimum ~ 0.5 angstroms, and our implementation failed to account for this.

Despite this error in our calculated results, our predicted results for ground state energy as a function of bond length match the expected results quite nicely. This suggests that our algorithm was on average able to estimate ground state energy with impressive accuracy, and would likely hold accurate if our algorithm accounted for the energy function around the turning point.

Method

In this project, our method is entirely computational. We work entirely with our implemented version of a VQE algorithm to test ground state energy at different bond lengths. We model our ansatz after the 'Scalable Quantum Simulation of Molecular Energies' journal by O'Malley et al. which employs the the Unitary Coupled Cluster (UCC) ansatz. Coupled Cluster takes the ground state $|\Phi\rangle$ and acts an exponential operator e^{-T} to obtain the excited state $|\Psi\rangle$: $|\Psi\rangle=e^{-T}|\Phi\rangle$. UCC is generally championed for its superior accuracy in semi-classical computational algorithms. This is built on the Hartree-Fock theory, which is the basis for many quantum chemistry eigensolver algorithms, and therefore lays the foundation for our experiment. Hartree-Fock solves for the wavefunction and energy of a system by splitting the general wavefunction into independent electron wavefunctions: $\Psi(r_1, r_2, \dots, r_N) = \phi_1(r_1)\phi_2(r_2) \dots \phi_N(r_N)$, where the interaction between electrons is added separately to the Hamiltonian (energy operator). The Hamiltonian we use to calculate our ground state energies is given by:

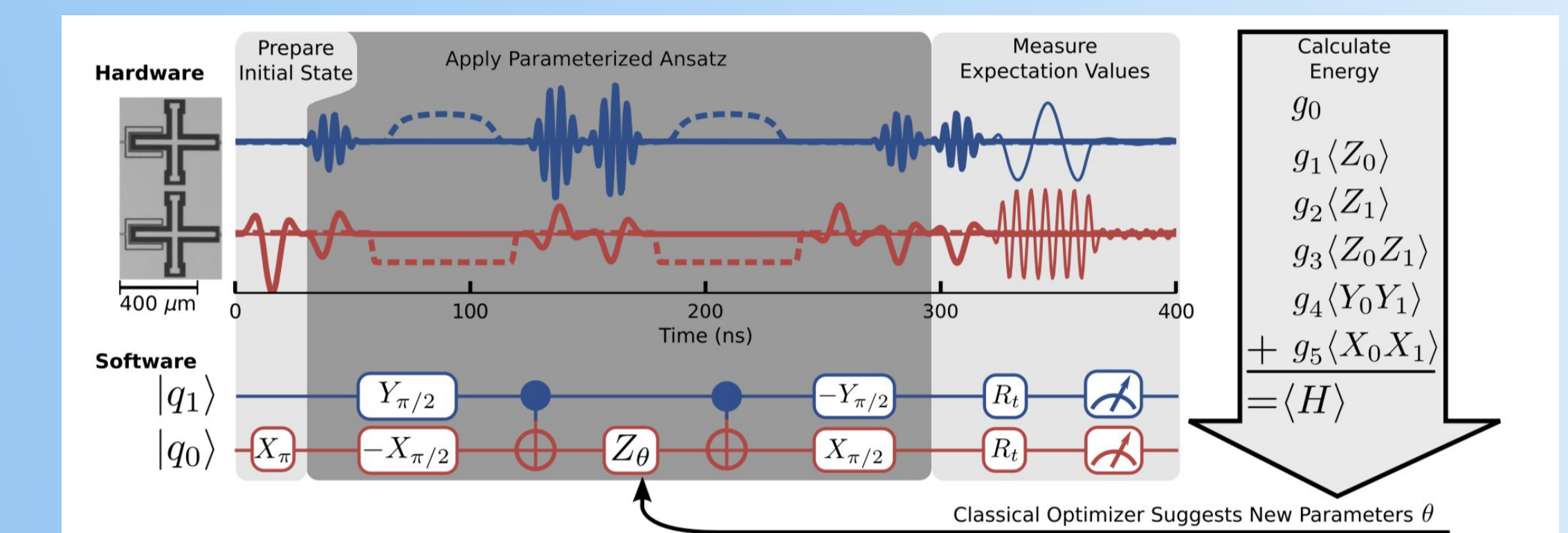


FIG. 1. Hardware and software schematic of the variational quantum eigensolver. (Hardware) micrograph shows two Xmon transmon qubits and microwave pulse sequences to perform single-qubit rotations (thick lines), dc pulses for two-qubit entangling gates (dashed lines), and microwave spectroscopy tones for qubit measurements (thin lines). (Software) quantum circuit diagram shows preparation of the Hartree-Fock state, followed by application of the unitary coupled cluster ansatz in Eq. (3) and efficient partial tomography (R_i) to measure the expectation values in Eq. (1). Finally, the total energy is computed according to Eq. (4) and provided to a classical optimizer which suggests new parameters.

where X, Y, and Z are Pauli spin operators.

Future Research

We restricted our focus to the dihydrogen molecule, and therefore were unable to run our experiment on Helium, or even hydrogen itself. Nonetheless, as a sort of efficacy check, a plan for future research could be running the same algorithm with variable bond lengths on hydrogen and helium.

Furthermore, one could ask: does the specific implementation for a 2-qubit system heighten the efficacy of the algorithm? Would it be beneficial to hardcode future algorithms for multi-qubit systems, rather than trying to work with a generalized algorithm?

Acknowledgements

We would like to thank the ULAB executives, faculty sponsor Prof. Dan Kasen, our mentor Sri, the Discovery Grant PI Prof. Eugene Chiang, and UC Berkeley for making this research opportunity possible.

Citations

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