ECE 592-081: Quantum Computing Semester Project B1 Description and Timeline

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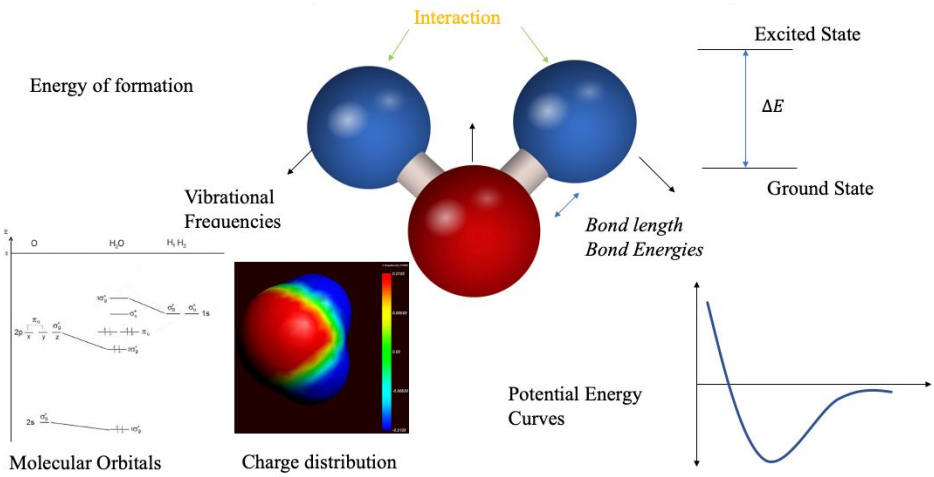
https://pages.github.ncsu.edu/wmccray/ECE592ProjectB1/

Quantum computing finds applications in solving classically large chemistry problems. It may help us solve problems such as high temperature superconductivity, catalysis, excited energy transitions and chemical reactions. Building a sufficiently large quantum computer will be a difficult challenge and recently developments have been made to tackle this problem using small quantum resources.



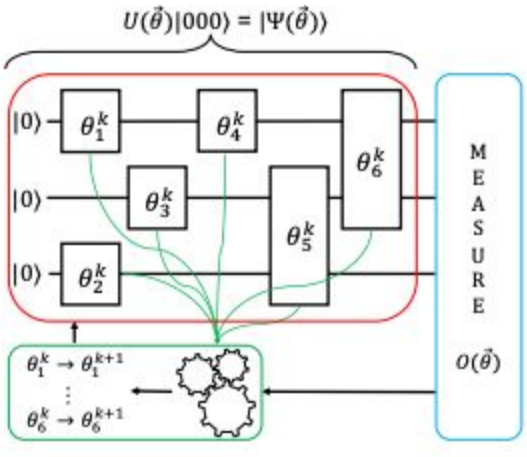
The way to approach this problem is to solve the adiabatic Schrodinger equation. The wavefunction in the Schrodinger equation is a complicated function of all the electronic and spin coordinates for the molecule. As the molecule increases in size the number of computations increases exponentially.

Many computation methods exist such as the Hartree-Fock method DFT, Multi-configurational self-consistent field CI method for evaluating ground as well as excited states.

A stepwise method to solve the problem is that we need to first encode the wavefunction as a form of basis sets. A wide variety of basis sets exist for different molecular systems limiting the accuracy and complexity of the system. The basis set is solved using the variational principle for the lowest energy state iteratively. This is where the quantum resource can be utilized.

To tackle this problem many Quantum Algorithms that have been developed and implemented:

1. Quantum phase estimation
2. Variational Quantum Eigensolver (shown in figure)
3. Evaluation of excited states



During this project we are going to design a custom quantum architecture that is well suited to solving computational chemistry problems. The design will have realistic constraints for the quantum hardware utilized. The cost and performance of the design will be measured by estimating the price to produce the hardware and estimating the performance of the hardware relative to hardware that already exists.

Timeline

Task	Date to Be Completed By
Submitted Description and Timeline	Oct. 8, 2020
Technical Review Completed	Oct. 15, 2020
Design Completed	Oct. 22, 2020
Final Report Completed	Oct. 29, 2020
Turn In Final Report	Nov. 17, 2020

Bibliography

Li, Gushu, et al. “Towards Efficient Superconducting Quantum Processor Architecture Design.” *ASPLOS*, 20 March 2020, https://asplos-conference.org/2020/program.html. Accessed 7 October 2020.

McArdle, Sam, et al. “Quantum computational chemistry.” *arXiv:1808.10402 [quant-ph]*, Rev. Mod. Phys. 92, 15003 (2020), 27 January 2020, https://arxiv.org/abs/1808.10402. Accessed 8 October 2020.