ECE 592-081: Quantum Computing Semester Project B1 Progress Report 1

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

Implementation of QisKit tutorial into simulation of ground state energy of LiH and comparing with actual implementation.
The following steps were implemented.

1. Define a molecule and get integrals from a computational chemistry driver (PySCF in this case)
2. Construct a Fermionic Hamiltonian and map it onto a qubit Hamiltonian
3. Instantiate and initialize dynamically-loaded algorithmic components, such as the quantum algorithm VQE, the optimizer and variational form it will use, and the initial_state to initialize the variational form
4. Run the algorithm on a quantum backend and retrieve the results

Over the next few weeks we will be simulating a Helium atom on QuisKit similarly to how the Hydrogen atom was simulated using the above method.

Task	**Contribution**
Literature Review	Kelvin and William Equally
Functions and implementation	Kelvin and William Equally
Task to be done	**Timeline**
Run on real device IBM Q	Oct 29, 2020
Perform additional research on **He** energy states	Nov. 5, 2020
Have draft of **He** atom simulation script complete	Nov. 12, 2020
Simulate with **He** atom	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.

Wood, Steve, and Manoel Marques. “qiskit-aqua.” *GitHub*, https://github.com/Qiskit/qiskit-aqua. Accessed 22 10 2020.