Step 1: Explain the technical problem you solved in this exercise

The main goal of this exercise was to use variational quantum eigensolvers (VQE) in order to solve for the ground state energies of four different molecules, H2, LiH, H4, and NH3 and compare with the results from classical quantum-chemistry algorithms. In particular, the Hartree-Fock **(HF)**, Coupled-Cluster Singles and Doubles **(CCSD)** as well as the full configuration interaction **(FCI)** methods.

In exercise 1: We solved the LiH, H4, N2, and NH3 molecules using classical quantum-chemistry algorithms. The potential energy surface plots of the three molecules as a function of the molecular parameters are plotted in Figures 1,2,3 and 4 below.

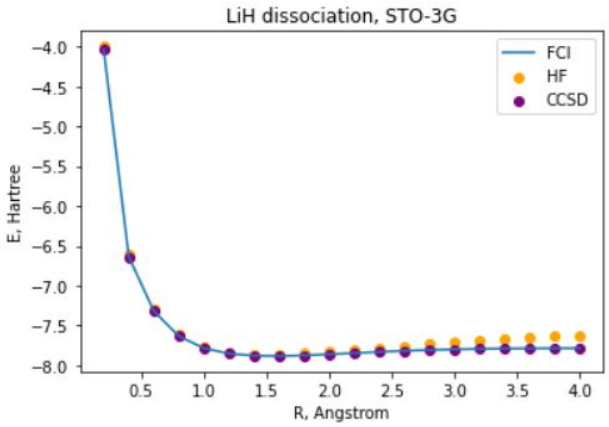

Figure 1: The LiH molecule solved using the FCI, HF and CCSD methods

In Fig. 1, the LiH molecule exhibits a smooth decreasing potential energy pattern for all algorithms considered. There is some disagreement between the CCSD energies and HF at larger distances due to the different approximations involved.

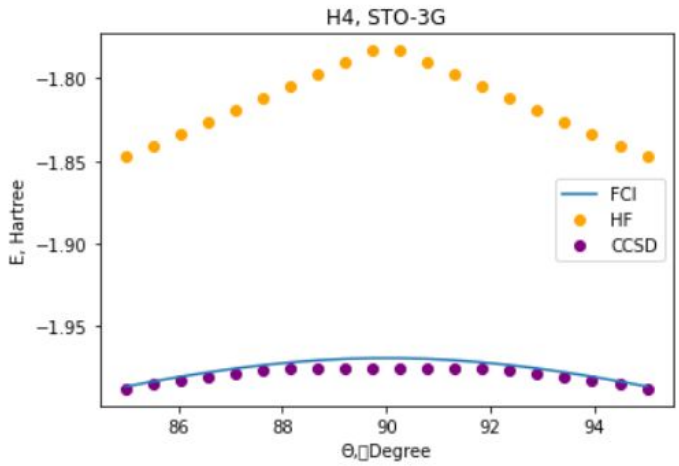

Figure 2: *The H4 molecule solved using the FCI, HF and CCSD methods*

The energy of the H4 molecule in Fig. 2 is plotted as a function of the molecular angles. Here, the HF method fails to get the correct energy-angle dependence. The FCI and CCSD methods generate nearly identical values.

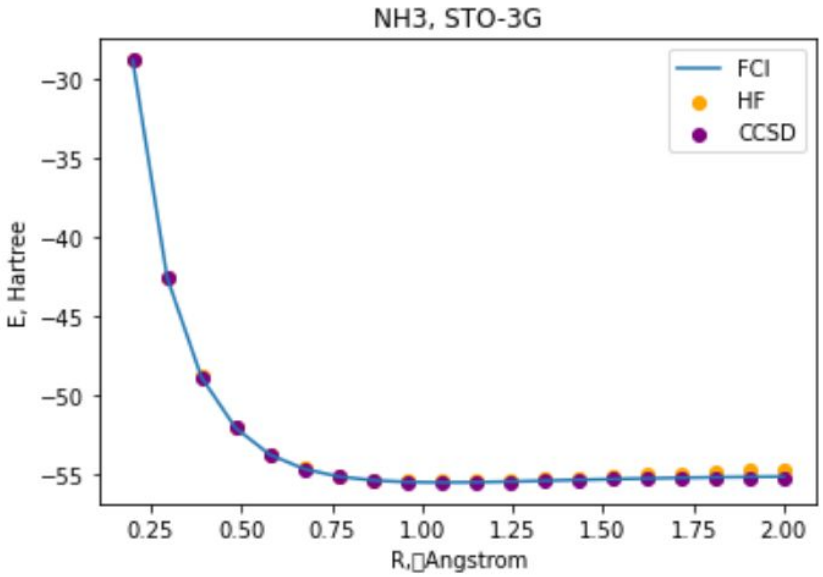

Figure 3: The NH3 molecule solved using the FCI, HF and CCSD methods

The potential energy surface generated by the HF and FCI algorithms smoothly decreases as a function of molecular distances. All methods agree for this molecule to high accuracies.

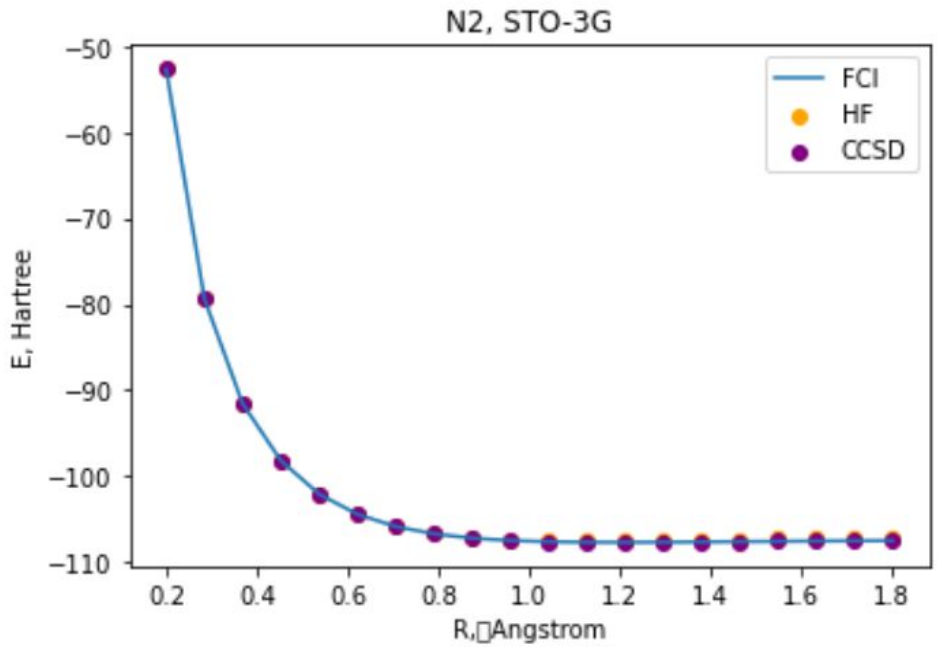

Figure 4: The N2 molecule solved using the FCI, HF and CCSD methods

The potential energy surface generated by the HF and FCI algorithms smoothly decreases as a function of molecular distances. All methods agree for this molecule to high accuracies.

In exercise 2: The qubit hamiltonians for H4, LiH, and NH3 is generated. We tried using the Jordan-Wigner transformation as well as using the Tapered Hamiltonians to reduce the size of the effective Hamiltonian. The effective Hamiltonians generated from this analysis are in our notebook. The energies obtained from the effective qubit Hamiltonians of the three molecules that we considered are given in Table 1.

Molecule	**Energy [Hartrees]**
H4	-1.96946153
N2	-107.549300
LiH	-7.78446028
NH3	-55.51550624532097

Table 1. The ground state energies from the effective qubit Hamiltonians for the different molecules considered.

In exercise 3: In this exercise, we employ the unitary coupled cluster (UCC) and the qubit coupled cluster (QCC) method, in order to generate Hamiltonians that can be implemented very efficiently as elementary unitary operators for several molecules (H4, LiH, N2, and NH3). Our results indicate that QCC is better that UCC in terms of speed.

In exercise 4: In this exercise, we use different methods to partition the effective Hamiltonian into several terms that can be partitioned into groups to be measured efficiently in quantum hardware. This method is demonstrated for H4, LiH, NH3, and N2.

In exercise 5: Using the entanglers and amplitudes determined in step 3, it is possible to find the corresponding representation of those operators as elementary gates using compilers. In this notebook, we carry out this procedure for several molecules of interest, H4, LiH, and NH3.

Step 2: Explain or provide examples of the types of real-world problems this solution can solve

Quantum chemistry has many applications for business. By modeling molecules as quantum-mechanical objects, it is possible to determine **reaction rates, molecular configurations, ionization energies, photon absorption spectra, vibrational modes**, and many other properties critical for the industry. The ability to solve quantum chemistry problems on a quantum computer may generate additional advantages gained.

Step 3: Identify at least one potential customer for this solution - ie: a business who has this problem and would consider paying to have this problem solved

The following drug discovery companies would find value from a quantum chemistry software with the advantage of quantum computing

- Protein Cure,
- Deep Cure,
- Atomwise.

Step 4: Prepare a 90-second video explaining the value proposition of your innovation to this potential customer in non-technical language

Our 90-second video proposal is given here:

https://photos.app.goo.gl/cuF58vTpbLHh9KbcA