Problem Statement

Contents

1 Quantum Chemistry

So the possible use cases for simulation of Quantum Chemistry can be simulation of energy eigenvalues of the molecules/polymers which are used in material synthesis. The electronic correlation problem.

We would be estimating the ground state energy eigenvalues of molecules by doing a imaginary time evolution(imaginary in the sense of complex no.) of the Hamiltonian operator of the molecule in question. The Quantum Monte-Carlo methods basically approaches the exact ground state of the Hamiltonian and "state" here basically is the vector i.e. we get to the eigen-vector for the ground state eigen-value, and using this when we can get a estimate of the ground state eigen values which is basically our motive i.e. ground state energy. We need to sampling of this guy obtained to get the final value of the energy.

We would be solving the molecules for H_4, N_2, and if possible for Diamond (we would see if this is feasible for us or not as it is really compilication system).

1.1 The Algorithm

You need to go through the article Unbiasing Fermionic Quantum Monte Carlo with a Quantum Computer Read the parts I have highlighted and uploaded in the github repository Your Task are as follows:

- First design the circuit for H_4 molecule given in Fig. 2 of the article, now this it self have several parts.
- First make the circuit of using the gates pre-given in the Fig. 2. Try to get an implemenation of basically Appendix C for this.
- Implementation of Shadow Tomography using Appendix D. You have to indentify which form of Gate combination would be a best fit for the problem.
- Get the measurement using the basis set used in the article to get the atomization energy.
- Repeat the same for N_2 by designing the Hamiltonian for it and using the idea given in Fig. 2.
- After this we would see if we can do the Diamond structure or not.