**Open Fermion**

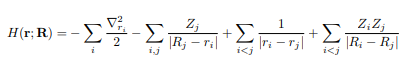
The project is about Quantum simulation of the molecules which is very widely used in molecular drug design by obtaining energy of molecule and other ground state parameters.

Firstly, we will see how a classical model works and then we see how is that implemented on a quantum computer. In classical model, we take the aid of Hartee-Fork ab-initio methods to get the ground state energy. We will use time dependent Schrodinger wave equation under the influence of Born-Oppenheimer approximation, which treats the nuclei as fixed point charges, and the ground state electronic energy is a parametric function of their positions That time dependent equation is

\begin{displaymath}
i \hbar \frac{\partial \psi({\bf r},t)}{\partial t} =
- \f...
...r^2}{2m} \nabla^2 \psi({\bf r},t) + V({\bf r}) \psi({\bf r},t)
\end{displaymath}`

Where Hamiltonian is sum of Potential energy and Kinetic energy.

In the HF method Hartee assumed many approximations and proceeded with slater type of orbitals (STO’s) and then Gaussian improvise the accuracy of these orbital calculations by considering Gaussian primitive function collectively known as basis set STO-3G. This type of approach is known as variational approach to solve the Schrodinger eigen value equation. For calculating Hamiltonian operator, we also consider Nuclei interaction and two electron integrals like Columbic integrals and exchange integrals. This combinedly is called as FOCK operator and orbitals obtained are fock orbitals.



We assume an exponential function(e-**µr2)**) as STO radial part and we proceed and obtain energy and we keep on correcting our wavefunction till the least energy that is experimental energy is obtained by modifying our wave function. This a classical approach of obtaining ground state parameters and bond energy graphs with respect to bond length.

Mapping Classical Hamiltonian to qubits:

So far, we have seen how a classical approach method works. Open Fermion is an open-source software library written largely in Python, aimed at enabling the simulation of fermionic models (electronic models as electrons are fermions) and quantum chemistry problems on quantum hardware. This platform is of great use and helps in simulating the classical method as described above from certain libraries like Pyscf and psi4. If we look in detail this platform maps classical information like Hamiltonian and wavefunction to qubits and converts them to Qubit operator through some transformation. Present quantum computers often work with distinguishable qubits as their computational units. To simulate indistinguishable fermionic particles, it is first required to map the fermionic state to the state of the qubits. This platform runs the piece of code for transformation on rigetti quantum virtual machine platform Forest. Upon this transformation, it gives Quantum circuit which gives the Qubit Hamiltonian.