**OpenFermion**

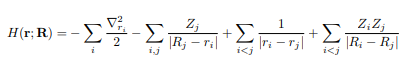
The project is about Quantum simulation of the molecules which is very widely used in molecular drug design by obtaining energy of molecule and other ground state parameters.

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.