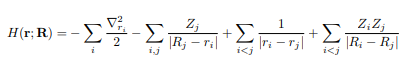
The project is about Quantum simulation of the molecules which is very widely used in molecular drug design by obtaining energy of molecule and other ground state parameters.

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.

OpenFermion requires certain energy calculations to be done before proceeding to the quantum computations so that these calculations form an initial guess. The calculations are done through various chemistry electronic structure packages such as PyScf and Psi4. Right now, there are plugins available for these both packages only.

This directory consists of classical energy calculations of the hydrogen molecule using the PyScf package. It performs certain Hartree-Fock calculations to do these calculations. The PyScf calculates the Molecular Hamiltonian and various density matrices.

We'll initialize a hydrogen molecule and calculate various energies such as Hartree-Fock energy, MP2 energy, FCI energy and orbital energies for the molecule at various bond lengths and plot the energies.

The minimum energy of the molecule corresponds to the bondlength of the molecule and the structure of the molecule.

Python libraries to be installed:

1. openfermionpyscf

2. pyscf