# Project 1 report: Hartree Fock with Integrals

Benjamin Peyton

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## 1 Overview

For this project, a code was developed according to the directions given in the Final Project 1 Description pdf. The code for the project spans across three files: *ints.py*, *hf.py*, and *opt.py*. The integral evaluation code is split into functions within *ints.py*, the Hartree Fock method is split into functions (and a total HF function is also implemented) within *hf.py* which calls on the integral functions from *ints.py* for the required integral matrices, and finally *opt.py* calls the HF procedure and uses it to perform a geometry optimization on $H_2$ using Newton-Raphson steps with approximated derivatives. The complete code can be found on my github page at github.com/bgpeyton/HF_Int along with a *README* which outlines the code and describes dependencies (math, numpy, and scipy packages).

## 2 Derivations and Procedure

Before integral evaluation, a closed expression for the integral in Eq (1) was derived to be used later for Gaussian-type integrals.

$$R_k = [integral]x^k e^{-\alpha x^2} dx \tag{1}$$

Next, using the Gaussian product theorem, a closed expression for the overlap integral between two primitive non-normalized Gaussians was derived. The function *gen_S*() was coded in *ints.py* to evaluate these overlap integrals, and another function *S_mat*() returns a matrix of such integrals given a molecule and basis set.

For kinetic energy integrals, again a closed form expression was derived. This expression was implemented in *gen_K*() within *ints.py* and then *K_mat*() generates a matrix of these integrals

given a molecule and basis set.

An expression for nuclear attraction integrals was given, and this was implemented as $gen\_V()$ within *ints.py* and followed by $V\_mat()$. Similarly, the expression for the electron repulsion integrals was given and implemented as $gen\_eri()$, followed by $eri_mat$ which returns the later-discussed $G$-matrix necessary for the Hartree Fock procedure.

# 3 Results