Homework-3

Due Date: April 13th, 5:00 PM.

Q1. Consider the PH_3 (Phosphine) molecule. If we decide to do a calculation on Phosphine and use the STO-3G basis set, how many contracted basis functions will we need to minimally represent the total number of atomic orbitals spanned by the core and valence electrons of the Phosphorus atom and the three hydrogen atoms? How many one-electron integrals will there be that require evaluation? How many two-electron integrals will require evaluation? In each of the last two cases, how many primitive integrals will need to be evaluated? Do you see anything that makes the workload slightly less onerous than your formal analysis? How many occupied orbitals will there be in the final Slater determinant?

Q2. What is the Hartree-product wave function for 2 non-interacting quantum mechanical harmonic oscillators (QMHOs) of reduced mass 1 a.u. in a potential having a force constant of 1 a.u., where the first QMHO is in the ground state and the second is in the first excited state? Determine the energy of the two QMHO system as an expectation value of the Hartree-product wave function. Is the correct Hamiltonian for this system separable into one-QMHO terms?