Problem Set 1

Show all work and provide clear explanations to receive credit.

1) Starting from the time-independent Schrodinger equation in differential equation form:

$$\hat{H}\Psi(r) = E\Psi(r)$$

insert the definition of the wave function as a sum over basis functions:

$$\Psi(r) = \sum_i c_i \phi_i(r)$$

Assuming that the basis is orthonormal, demonstrate that the Schrodinger equation can be rewritten in matrix form:

$$\mathbf{H}\vec{c} = E\vec{c}$$

with the elements of the Hamiltonian matrix, $\mathbf{H}$, defined:

$$H_{ij} = \int \phi_i(r)\hat{H}\phi_j(r)dr$$

2) How many contracted Gaussian basis functions are in the following basis sets for the following atoms or molecules. (Show work by listing all basis functions in each case.)

a) 3-21G, hydrogen atom

b) 6-31G**, carbon atom

c) aug-cc-pVDZ, carbon atom

d) 6-31+G, a molecule of ethene (C_2H_4)

3) Write a Slater determinant for the ground state of the Helium atom. (Use $\phi_{1s}(r)$ and $\overline{\phi}_{1s}(r)$ to represent the spin up and spin down 1s spin orbitals, respectively; use r_1 and r_2 to represent the coordinates of electron 1 and 2, respectively.) Show that this wave function is antisymmetric with respect to exchange of the electrons.