MEST - Assignment 1

(For each solution, show your work through a set of important steps)

Operation Complexity

1. For an array containing N integers, derive the number of operations required to
   a) obtain the maximum value in the array.
   b) sort the integers in a descending pattern. (2+ 2 pts)

2. Hartree-Fock (HF) is one of the methods to calculate total energy of the molecule. The HF energy expression is:

$$E^{HF} = \sum_{i}^{N_{occ}} \int \chi_i(x_i)\,\hat{h}\chi_i(x_i)\,dx_i + \frac{1}{2}\sum_{i=1}^{N_{occ}}\sum_{j=1}^{N_{occ}} \int dx_i x_j \chi_i(x_i)\,\chi_j(x_j)\,\frac{1}{\hat{r}_{12}}\chi_i(x_i)\,\chi_j(x_j)$$

$$-\frac{1}{2}\sum_{i=1}^{N_{occ}}\sum_{j=1}^{N_{occ}} \int dx_i x_j \chi_i(x_i)\,\chi_j(x_j)\,\frac{1}{\hat{r}_{12}}\chi_i(x_j)\,\chi_j(x_i)$$

   Where, $\chi(x)$ are the space-spin molecular orbitals with space-spin coordinate x, $\hat{h}$ is one electron Hamiltonian and $\hat{r}$ is the interelectron distance and N_{occ} denotes the occupied molecular orbitals respectively. Suppose we have a H_2O molecule with a total of 10 space-spin molecular orbitals.

   (a) Calculate number of one electron and two electron integrals required to compute HF energy of a single H_2O molecule. (3 pts)

   (b) If each one-electron and two-electron integral require 5 and 10 floating point operations respectively, and a given processor can do 45 giga floating point operations per second (45 GFLOPS), then calculate the time required to compute Hartree-Fock energy of (3 pts)

      i. a single H_2O molecule
      ii. $(H_2O)_4$ cluster
      iii. $(H_2O)_N$ cluster

Spin, Spin matrices, Pauli exclusion prinicple

1. Discuss the experimental setup for a Stern-Gerlach experiment. Why does the beam consisting of neutral (e.g. Ag) atoms is split into different beams? (3 pts)

2. Prove the following relations (1+1+1+1+1 pts):

   (a) $S_+S_- = S^2 - S_z^2 + S_z$

   (b) $S_-S_+ = S^2 - S_z^2 - S_z$

(c) $[S_+, S_z] = -S_+$

(d) $[S_-, S_z] = S_-$

(e) $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$

3. An electron is in the spin state

$$A = \begin{bmatrix} -8i \\ 15 \end{bmatrix}$$

(a) Find the expectation values of $S^2, S_z, S_+, S_-, S_x, S_y$ operators. (3 pts)

(b) Find the root-mean-square deviations $\Delta S_z, \Delta S_x, \Delta S_y$. (3 pts)

4. Derive the S_+ and S_- operator matrices for a spin-1/2 ($m_s = -1/2, 1/2$) system. (2 pts)

5. Derive the $S^2, S_z, S_+, S_-, S_x, S_y$ operator matrices for a spin-1 ($m_s = -1, 0, 1$) system for which the spin states are given by (6 pts)

$$a = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, b = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \; c = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$