Exercise Ex4

Student: Firstname Lastname Sciper: 000000

**Please use this template to submit your answers.**  
If you had to modify code from the notebook, please include the modified code in your submission either as screenshot or in a

\begin{lstlisting}[language=Python]  
\end{lstlisting}

environment.

You only need to include the code cells that you modified.

Note, that references to other parts of the documents aren’t resolved in this template and will show as ??. Check the text of the exercises on website for the reference

**Exercise 1**  
Define using Dirac notation.

Your answer here

**Exercise 2**  
For an orthonormal basis, what does the overlap integral array, S, look like?

Your answer here

**Exercise 3**  
Use B and B\_dagger and the matrix rules above to calculate the matrix S.

Your answer here

**Exercise 4**  
Describe how the notation of the np.einsum command correlates to the implicit summation formula written above.

Your answer here

**Exercise 5**  
Use the function np.einsum() to calculate the matrix S, and confirm that your answer is the same as above.

Your answer here

**Exercise 6**  
Propose a different orthonormal basis, modify phi1 and phi2, and verify that S still has the same form. There are infinitely many choices. It isn’t complex... or *is* it?!

Your answer here

**Exercise 7**  
How many electrons are there in total in H2O? How many occupied molecular orbitals would you expect?

Your answer here

**Exercise 8**  
Explain the shape (number of rows and columns) of S in terms of the AO basis set we chose.

Your answer here

**Exercise 9**  
Based on your observations of S in the AO basis, answer the following questions

1. What do the diagonal elements of S indicate?
2. What do the off-diagonal elements of S indicate?
3. Does the Gaussian atomic orbital basis set form an orthonormal basis?

Your answer here

**Exercise 10**  
Does the result of your extra evaluation agree with what you determined previously?

Your answer here

**Exercise 11**  
Use the function np.linalg.inv() to calculate the inverse of S, and the function splinalg.sqrtm() to take its (matrix) square root. Execute the code below and examine the matrix A.

Your answer here

**Exercise 12**  
What do you observe about the elements of A? Is the matrix real or complex? Is the matrix symmetric or not?

Your answer here

**Exercise 13**  
Use the orthogonalization matrix A to transform the overlap matrix, S. Check the transformed overlap matrix, S\_p, to make sure it represents an orthonormal basis.

Your answer here

**Exercise 14**  
The product A S A does not take the complex conjugate transpose of A. What conditions (properties of A) make that ok?

Your answer here

**Exercise 15**  
Based on the definition of , propose a definition of in terms of and . Justify your equation.

Your answer here

**Exercise 16**  
In the cell below, use the core Hamiltonian matrix as your initial guess for the Fock matrix. Transform it with the same A matrix you used above. To calculate the eigenvalues, vals, and eigenvectors, vecs, of matrix M using vals, vecs = np.linalg.eigh(M).

Your answer here

**Exercise 17**  
Display, i.e., print, the coefficent matrix and confirm it the correct size

Your answer here

**Exercise 18**  
Use A and the formula you proposed previously to transform the coefficient matrix back to the AO basis. Confirm that the resulting matrix appears reasonable, i.e., similar size and magnitude

Your answer here

**Exercise 19**  
Build the density matrix, D, from the occupied orbitals, C\_occ, using the function np.einsum(). **Hint** Look at ([[DensityMatrix]](#DensityMatrix))

Your answer here

**Exercise 20**  
Define J in terms of the density matrix, D, and the electron repulsion integral tensor, I, using np.einsum().

Your answer here

**Exercise 21**  
Define K in terms of the density matrix, D, and the electron repulsion integral tensor, I, using einsum().

Your answer here

**Exercise 22**  
Define F in terms of H, J, and K. (Recall The Hartree-Fock procedure)

Your answer here

**Exercise 23**  
Calculate the SCF energy based on H, F, and D using np.einsum().

Your answer here

**Exercise 24**  
Based on the result of the calculation in [[basisset]](#basisset), is this a reasonable answer?

Your answer here

**Exercise 25**  
Describe a procedure (i.e. identify the steps) that will update coefficients and compute a new density matrix based on the updated values of the Fock matrix.

Your answer here

**Exercise 26**  
Using the procedure proposed above, calculate the updated coefficients

Your answer here