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Homework assignment

Due Date: 02/28 by 11:59 pm

Fill in your solutions in the Pluto notebook provided below. Once completed, execute the notebook and export it as a PDF. Upload the PDF to Gradescope for grading, and assign the pages to the respective exercises. Please ensure that all of your solutions, including the code you wrote, are visible and legible in the exported PDF before submitting it to Gradescope. Keep in mind that adjustments to assignments after the submission deadline will not be accommodated.

Conceptual Problems

Exercise 1:

Determine the electronic configuration of nickel.

Solution:

Your solution goes here ...

Exercise 2:

Compute the one-body part of the electron-nucleus attraction for Slater determinants, i.e.,

$$V_{\text{en}} = \langle \Psi | \sum_{i=1}^{N} \sum_{j=1}^{N_{nuc}} \frac{Z_j}{\|R_j - r_i\|} | \Psi \rangle = \sum_{i=1}^{N} \langle \phi_i | \sum_{j=1}^{N_{nuc}} \frac{Z_j}{\|R_j - r\|} | \phi_i \rangle$$

Solution:

Your solution goes here ...

Exercise 3:

Given the spin-generalized Fock matrix, derive the spin-restricted Fock matrix, i.e.,

$$F[D] = T + V_{\text{en}} + V_J[D] - \frac{1}{2} V_K[D]$$

where

$$[V_J[D]]_{k,l} = \sum_{i,j} v_{ijkl} D_{ji}$$

and

$$[V_K[D]]_{i,l} = \sum_{j,k} v_{ijkl} D_{jk}.$$

Solution:

Your solution goes here ...

Programming Problems

Exercise 4:

Given the integral files T, $V_{\rm en}$, and v in files/equi_geom, write a function that computes the spin-restricted Fock matrix.

```
md" #### Exercise 4:
Given the integral files $T$, $V_{\rm en}$, and $v$ in files/equi$\_$geom, write a function that computes the spin-restricted Fock matrix.

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```

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compute_Fock_matrix (generic function with 1 method)
```

```
function compute_Fock_matrix(T::Matrix{Float64}, V_en::Matrix{Float64}, eri::Matrix{Float64}, dm::Matrix{Float64})
    # Your code goes here ...
    return F
end
```

Verify your code by comparing with Fock_matrix_1.4.npy in equi_geom

```
# Your code goes here
```

Exercise 5:

Using the overlap matrices in files/equi_geom, write a self-consisten field iteration method.

```
# Your code goes here
```

Verify your implementation by initializing your code with zero and comparing your output to rdm1_1.4 in equi_geom.

Report your convergence as a difference function per iteration.

```
# Your code goes here
```

Exercise 6:

Write a routine that performs RHF for the full potential energy surface of LiH. Use the data provided in files/PES.

```
# Your code goes here
```

Plot your computed potential energy surface and compare with the data provided in files/PES.

```
# Your code goes here
```