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Homework assignment

Due Date: 03/24 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:

Prove that

$$\langle \Psi_0 | V | \Psi_0 \rangle = \frac{1}{2} \sum_{i,j \in [N]} \langle ij || ij \rangle$$

```
# Your solution goes here
```

Exercise 2:

Following the notation in class, prove that

$$\sum_{i \in [N]} \varepsilon_i = \sum_{i \in [N]} \left(h_{ii} + \sum_{j \in [N]} \langle ij || ij \rangle \right)$$

```
# Your solution goes here
```

Exercise 3:

Prove that

$$\langle i | V_{\text{eff}} | a \rangle = \sum_{j \in [N]} \langle ij || aj \rangle$$

```
# Your solution goes here
```

Programming Problems

MP2 calculations for LiH

Exercise 4:

Given the AO integral files v and the MO energies in files/equi_geom, write a function that computes the spin-restricted MP2 correlation energy.

```
# Your code goes here
```

Verify your implementation by comparing your output to mp2_ecorr_1.4 in equi_geom.

```
md"
Verify your implementation by comparing your output to mp2$\_$ecorr$\_$1.4 in
equi$\_$geom.
"
```

```
# Your code goes here
```

Exercise 5:

Write a routine that performs spin-restricted MP2 for the full potential energy surface of LiH. Use the data provided in files/PES.

```
md" #### Exercise 5:
Write a routine that performs spin-restricted MP2 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 reporting the total energy and compare with the data provided in files/PES. In addition to the MP2 energy include a plot of the RHF energies, comapring the two theories.

```
# Your code goes here
```