FYS-4096 Computational Physics: Exercise 7

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Week 10

General:

- You should have access to `ex7_help` on teacher's repo.
- There you will find files `hartree_1d.py` and `h5_help.py` that will most likely be useful in this exercise.
- **Deadline always before noon on Monday the following week!** That is, for these problems before noon on Monday March 15.

Problem 1: 1D harmonic quantum dot with N interacting electrons

- Write a simple code that solves the Schrödinger equation of N interacting electrons in 1D harmonic quantum dot using the Hartree approximation.
- Approximate the Coulomb interaction in 1D as

$$V_{1D}(x) = \frac{a}{\sqrt{x^2 + b}}. \tag{1}$$

- For testing use $a = b = 1$, $N_e = 4$, and all electrons have up-spins, i.e., populate orbitals with different orbital quantum numbers. (Notice that setting $a = 0$ would give you the non-interacting case.)
- Remember that the electron density is given as $n(x) = \sum_i |\phi_i(x)|^2$.
- Hint: Modify the `hartree_1d.py` where needed. When it is working you should get the values provided in the beginning of the file.
- Remember to **comment the code** in order to increase everyones understanding, and make a proper plot of the electron density. Include the energetics into the figure, and make the figure more presentative than currently.

Problem 2: Text file initialization and output

- Modify your code of problem 1 to provide output in text files. This should include orbitals, electron density, grid, etc.
- Further modify the code so that you can continue the run from where it finished (cleanly) last time. That is, the code should be able to read existing files with orbital, density, etc. related data that it will use in the intialization of the new run. For example, instead of tolerance of 0.01 you want to push the calculation a bit further upto tolerance of 0.00001.
- Test your code, for example, with the two different tolerances.
- Some help may already be available in the example code file.

Problem 3: HDF5 file initialization and output

- Modify the code of problem 1 in the same way as in problem 2, but using the HDF5 file format. (It is very convenient format, especially for large amount of transferrable data.)
- Test your code, for example, with the two different tolerances mentioned in Problem 2.
- Some help may already be available in the `h5_help.py` file.

Problem 4: Six electrons in 1D harmonic quantum dot

- Use your code that can provide output in either text or HDF5 format. That is, either problem 2 or problem 3 needs to be done before this problem!
- Calculate the Hartree ground state $S = 0$ and excited state $S = 3$ for six electrons in a 1D harmonic quantum dot with $\omega = 1$.
- Compare the energetics and electron densities.
- Plot the electron densities in a same figure. You can also add energetics into the figure in order to have all the comparisons easily available.
- How much do the energies change compared to the non-interacting case for both $S = 0$ and $S = 3$ states?
- How many SCF iterations are needed for the non-interacting case calculations?

Returning your exercise

1. Make a new folder "exercise7" to your existing Computational Physics repo.
2. Into the folder "exercise7" write a file "solvedProblems.txt" with a comma separated list of problems you have solved, e.g., 1,3,4x.
3. Make sure all your source files and related figures are under version control and push them to GitLab.
4. Push your commits to GitLab before noon on Monday March 15:
   ```
   git push --all && git push --tags
   ```