FYS-4096 Computational Physics: Exercise 11

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Week 15

General:

- You should have access to `ex11_help` on teacher's repo.
- There you will find, e.g., files `pimc_simple.py`, and `spin_mc_simple.py` that will most likely be useful in this exercise.
- **Deadline before noon on Monday the following week!** That is, for these problems before noon on Monday April 19.

Problem 1: Nearest neighbor spin model for ferromagnet.

- Modify `spin_mc_simple.py` or make your own classical Monte Carlo code for solving the Ising model with nearest neighbor interactions.
- For the example code you need to add, e.g., the Metropolis Monte Carlo algorithm for flipping a spin. There should read `# ADD` where something needs to be added.
- Add comments for better understanding (especially for all the `# ADD` parts).
- With the default settings you should get roughly -0.8 (in the used units) as your total energy per spin (once the code is working correctly).
- What are the default settings (in the used units): temperature, grid size, dimensions of the system, boundary conditions, and exchange constant?

Problem 2: Adding observables

- Include the calculation of heat capacity (C_V), magnetization (M) and magnetic susceptibility (χ) in to the code of problem 1.
- With the default settings you should get roughly the values 0.4, 0.0, and 0.3 for the previous (again per spin values). See that these work before continuing.
- Plot the behavior of these observables as a function of "Monte Carlo" time, i.e, as a function of block averages. Include the estimate for the observable into the plot. Include the figure(s) in your repository (as pdf or png).

Problem 3: Temperature effects and phase transition

- Calculate all the observables (E, C_V, M, and χ) as a function of temperature, e.g., for $T \in [0.5, 6.0]$ Kelvin.
- Make plots of the ensemble averages as a function of temperature. You should get similar curves as shown in Fig. 1.
- You should see signatures of phase transition in your figures. What is roughly the transition temperature?

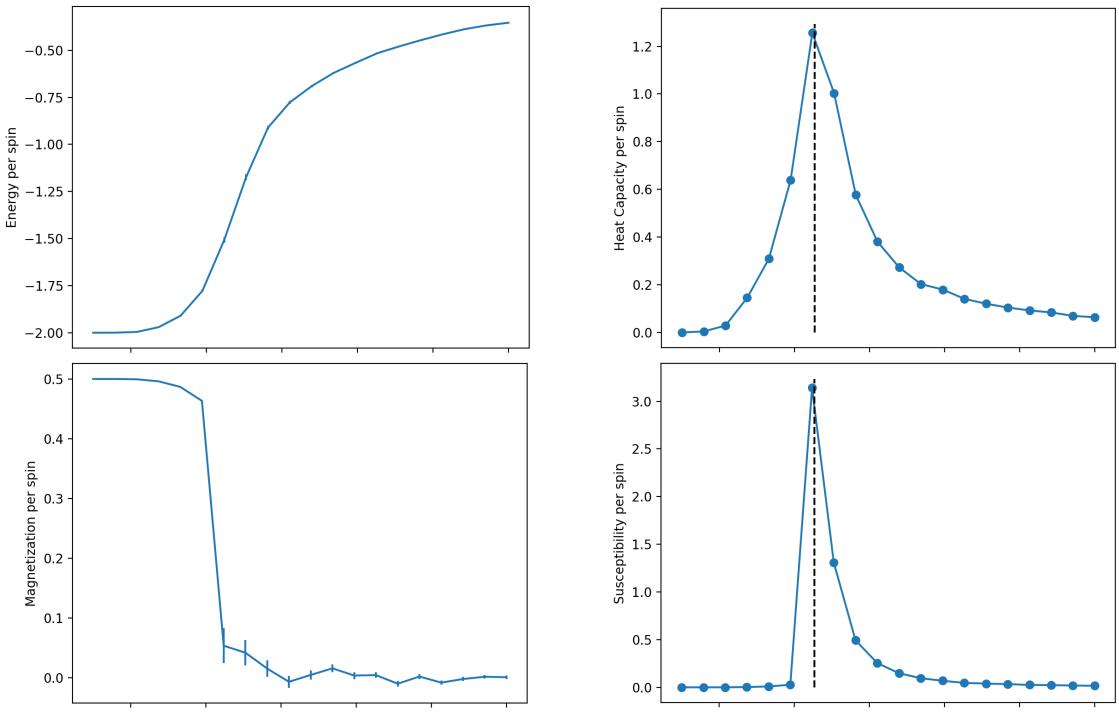

Figure 1: Observables as a function of temperature. Temperature values are intentionally not shown.

Problem 4: Classical vs. quantum atoms

- Modify your path integral Monte Carlo code or code a new one: the goal is to simulate two hydrogen atoms in 3D interacting via Morse potential energy surface. Use Morse parameters from the lecture slides.
- Compare energetics and internuclear distance for classical and quantum atoms, i.e., Trotter numbers $M = 1$ (classical) and quantum $M \to \infty$. For the quantum case consider for example, $M = 8$ and $M = 16$. Use $T = 300$ Kelvin, that is, roughly the room temperature.
- Make figures of the comparisons, and include those into your repository.
- The mass of a proton in atomic units is roughly 1836.
- Notice: You can use the "electrons" in the current code as your protons. Then you just need to change the mass in all relevant places, and see that you do not use the "nuclei" of the current code anywhere. If proper particle properties are given, then the code modified this way considers the "electrons" of the code to be atoms (protons).

Returning your exercise

1. Make a new folder "exercise11" to your existing Computational Physics repo.
2. Create a file solvedProblems.txt in the "exercise11" folder. Inside it, write a comma separated list of problems you have solved, e.g., 1,2,3.
3. Make sure all your source files and relevant figures are under version control and push them to GitLab.
4. Push your commits to GitLab before noon on Monday April 19:
   `git push --all && git push --tags`