Report problem

Report problem 1-1: Auto-correlation functions

- Calculate auto-correlation functions of relevant observables as follows

1. Select your model.
   - For example, you may choose Ising model on square lattice. Instead, you may choose LJ particles.
   - If you do not have a particular preference, I recommend the Ising model because it is one of the simplest examples.
2. Perform MCMC or MD simulation for the model.
   - In the case of the Ising model, you may perform MCMC simulation. For LJ system, you may perform MD or MCMC.
   - Don't forget to mention the algorithm you used.
3. Calculate auto-correlation functions of, at least, two observables in equilibrium.
   - For Ising model, they may be magnetization, squared magnetization, or energy.
     - In this case, please notice a difference between the magnetization and its square (or its absolute value).
   - For LJ particles, they may be the potential energy, the temperature or pressure.

Report problem 1-1: Auto-correlation functions

4. **Discuss** behaviors of auto-correlation functions and correlation time by varying temperatures (or similar relevant quantity) and system sizes (# of particles).
   - Please consider in what cases the correlation time will be longer.
   - Please include a discussion about *how we should set simulation time (MC steps)* to obtain reliable data when the correlation time will be longer.
     - Remember the relationship between the correlation time and the statistical error.
   - It might be useful to see the integrated correlation time

$$\tau = \int_0^\infty \frac{C(t)}{C(0)} dt \sim \sum_{t=0}^{T} \frac{C(t)}{C(0)}.$$

5. (optional) Change algorithm and compare correlation times among them.
   - For Ising model, you may consider, Metropolis, heat bath or cluster algorithms.
   - For MD, it might be interesting to see the difference among ensembles, although you may not see significant difference.

Report problem 1-1: Tips

- For MCMC or MD simulation, you can use
  - Your own code
  - Open source softwares
  - My sample codes (python) (Ising-auto.ipynb or .py, and LJ-auto.ipynb in Report1.zip).
    - In order to run the sample codes, you need numpy, matplotlib, and numba modules in addition to the python3.
    - See also the header of the codes.
- In order to obtain correct auto-correlation function, we need to take care about "thermalization" (initial state dependence) mentioned in the lecture.
  - In the case of the sample codes of Ising model,
    When you increase the system size
    or
    when you change the temperature,
    you may need to increase the "thermalization" parameter, which sets
    MC steps discarded before calculating auto-correlation functions.
  - It is also important to sample sufficiently long time, to evaluate the correlation time.

Report problem 1-2: Square lattice Ising model

- Investigate phase transition of the square lattice Ising model as follows

1. Perform MCMC for at least three system sizes. It is recommended to include larger than L=32 (e.g. L=48, 64, …), if your computer environment allows it. Otherwise, simulation up to L=32 is also acceptable.
   - Please explicitly write down the algorithm you used, e.g., Metropolis, Heatbath, Swendsen-Wang, ...
2. Plot, at least, magnetization^2 and specific heat as functions of temperature.
   - Note: Temperature range should contain the critical temperature.
3. **Discuss** the behavior of the error bars of the above quantities when you vary the MC steps, L and temperatures.
4. Plot the “binder ratio of magnetization” and estimate crossing point of them.
   - Don't forget to compare it to the expected value.
5. Try finite-size scaling of the binder ratio by using the exact and slightly different critical exponents.
   - By changing the horizontal axis properly, you will see a data collapse independent on L.
   - (optional) Try finite size scaling of magnetization^2.
6. (optional) Try cluster algorithm and compare the error bars with those in local updates.

Report problem 1-2: Tips

- For MCMC simulation, you can use
  - Your own code
  - Open source softwares, such as ALPS.
  - My sample codes (python) (Ising-obs.ipynb or .py in Report1.zip).
    - In order to run the sample codes, you need numpy, matplotlib, and numba modules in addition to python3.
    - See also the header of the codes.
- In order to obtain accurate results corresponding to the thermal equilibrium, MC steps are so important.
  - As I mentioned in the lecture, e.g., when the thermalization is too short compared with the correlation time, your result may be biased by the initial condition.
    - Note that even if the thermalization is sufficient, the statistical error also depends on the correlation time.
  - As you will experience in the report problem 1-1, the correlation time depends on the temperatures and the system sizes.

Report problem 1-2: about ALPS

- In case you use ALPS, **simplemc** and **spinmc** are the applications suitable for the report problem 1-2.
  - The tutorial mc-09 is highly related to the report problem.
  - If you want to use ALPS, please contact me. I can provide a sample input file for the report problem 1-2.
- Note that several quantities have different names in **simplemc** and **spinmc**.

	simplemc	spinmc
<E>	Energy Density	Energy Density
<M²>	Magnetization Density^2	Magnetization^2
<C>	Specific Heat	Specific Heat
binder ratio	Binder Ratio of Magnetization	Binder Cumulant

* In the case of *simplemc*, the definition of Binder ratio is reversed from that of *spimc,* which was presented in the lecture No. 4.

Important notice

- Please check that you can perform the report problem in your environment, as soon as possible.
  - I recommend google colab to run my sample codes.
    - Please see a short instruction in the No.4 slide.
    - If there is a trouble to try the report problem, please contact me at the lecture or by email.
- "(Optional)" indicates that they are not mandatory, although you will get extra points when you include them in your report.
- If a report contains only figures, you will loss lots of points.
  - Please include *explanations* and *discussions* about your results. These are essential!

Deadline

- Submit your report through the system of ITC-LMS
  - The tentative deadline is 2021 July. 13th.
    - It might be updated in the future.
      Don't forget to check the most up-to-date information.
  - In case you cannot use ITC-LMS, please submit it by email.
    - I will send reply when I receive your reports.
    - If you will not receive any response, please contact me.
- If you have any troubles or questions, please freely ask me
  - at the future lectures,
  - by email: t-okubo@phys.s.u-tokyo.ac.jp
  - or come to my office **Sci. Bldg. #1 940.**
    (It is better to get an appointment by email.)