Report problem 1-1: Auto-correlation functions

- Discuss the auto-correlation function and its relaxation time as follows

1. Perform MCMC simulation of the square lattice Ising model.
    - Don't forget to mention the algorithms you used. They may be Metropolis, heat bath, Swendsen-Wang (cluster), …
    - If you prefer, you may simulate another model, such as MCMC simulation of cubic lattice Ising model, MD simulation of LJ particle, …
2. Calculate (and plot) auto-correlation functions of magnetization (<M>) and squared magnetization (<M^2>).
    - When you select a different model, please choose your observables accordingly.
3. **Discuss** behaviors of auto-correlation functions and correlation time by varying temperatures and system sizes (# of spins).
    - Please discuss in what cases the correlation time will be longer.
        - Note that when the system size is too small, you may not observe explicit parameter dependences.
    - Please discuss the differences between <M> and <M^2> correlation times.

Report problem 1-1: Auto-correlation functions

4. Based on the previous discussion, consider how we should set MC steps (simulation time) to obtain reliable data when we change temperature and system size.
    - Remember the relationship between the correlation time and the statistical error.
5. (optional) We may reduce (or increase) the correlation time if we choose a different algorithm. Try MCMC simulation with another algorithm and compare the correlation time with the original algorithm.

Note:

To discuss the correlation time, it might be useful to use the integrated correlation time defined as

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

Report problem 1-1: Tips

- For MCMC simulation, you can use
  - Your own code
  - Open-source software
  - My sample codes (python) (Ising-auto.ipynb or .py 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 the “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: Phase transition

- Investigate the phase transition of the $L \times L$ square lattice Ising model as follows.
  1. Perform MCMC for at least three system sizes, such as L=16, 32, and 64. If your computer environment allows, it is recommended to include larger than L=32 (e.g., L=48, 64, …).
     - Please explicitly write down the algorithm you used, e.g., Metropolis, Heatbath, Swendsen-Wang, ...
  2. Plot the figures of the squared magnetization and the specific heat as functions of temperature. (You can also include figures of other quantities.)
  3. Try to (roughly) estimate the transition temperature, T_c, from the behaviors of specific heat and the square magnetization.
     - Please note the expected behaviors in the thermodynamic limit (infinite L limit).
       - The specific heat diverges at T_c.
       - The magnetization is zero and finite when $T > T_c$ and $T < T_c$, respectively.

Report problem 1-2: Phase transition

4. Next, plot the "binder ratio of magnetization" and estimate the crossing temperature.
    - As explained in the lecture, this crossing temperature becomes an accurate estimate of T_c.
5. **Discuss** the above estimations of T_c.
    - Please compare them to the exact value of T_c. (You can find it in the lecture slide).
    - Please don't forget to mention the statistical errors.
6. Try the finite-size scaling of the binder ratio by using your estimate of T_c.
    - You may see a data collapse independent of L by adequately changing the horizontal axis. (As explained in the lecture, we need the critical exponent ν. Here you can use its exact value $\nu=1$, or you may estimate it from the data collapse.)
7. (optional) Try finite-size scaling of magnetization^2 and estimate the other critical exponent η.

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
<M^2>	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.*

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 trouble trying the report problem, please contact me at the lecture or 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 lose 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 2022 July. 31st.
    - It may 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 a reply when I receive your reports.
    - If you do not receive any response, please contact me.
- If you have any troubles or questions, please ask me
  - at the future lectures,
  - by email: t-okubo@phys.s.u-tokyo.ac.jp
  - or come to my office **Sci. Bldg. #1 950.**
    (It is better to get an appointment by email.)