Project 4.
Phase transition in the Ising model.

1. Ising model on the ring.

The energy of the Ising model on a ring is

$$E = -J\sum_{n=1}^{N} S_n S_{n+1} - H\sum_{n=1}^{N} S_n \,, \qquad (1)$$

where $S_n = \pm 1$ and $S_{N+1} \equiv S_1$. The energy of spin S_n interacting with nearest-neighbouring spins in a magnetic field *H* is

$$E_n(S_n) = -JS_n(S_{n-1} + S_{n+1}) - HS_n \qquad (2)$$

Choose *J* =1 as the energy unit. Use the Metropolis algorithm and find the temperature dependence of the magnetization.

Metropolis algorithm.

The Metropolis algorithm can be summarized in the context of the simulation of a system of spins as follows.

1. Establish an initial microstate. It is convenient to use all spins up in the initial state, since it takes less computational time. One also can use a state when spins take at random the values ± 1. However, this initial state takes more computational time.
2. Choose a spin at random and flip it, i.e., $S_n^{(new)} = -S_n^{(old)}$.
3. At given *T* and *H* compute

$$\Delta E_n = E_n(S_n^{(new)}) - E_n(S_n^{(old)}) \,. \qquad (3)$$

   This is the change in the energy of the system due to the flip of the spin *n*.
4. If ΔE_n is less than or equal to zero, accept the new microstate and go to step 8.
5. If ΔE_n is positive, compute the quantity $w = e^{-\beta \Delta E_n}$ where $\beta = 1/T$.
6. Generate a random number *r* in the unit interval [0, 1].
7. If $r \le w$, accept the new microstate; otherwise retain the previous microstate.
8. Determine the value of the desired physical quantities. Let it be the magnetization

$$M^{(a)} = \frac{1}{N}\sum_{n=1}^{N} S_n^{(a)} \,. \qquad (4)$$

Here the index *a* numbers the microstates.

9. Repeat steps (2) through (8) to obtain a sufficient number of microstates.
10. Periodically (after 100 new microstates) compute averages over the microstates. Skip first 100 microstates because the system is far from equilibrium.

$$< M >= \frac{1}{m}\sum_{a=1}^{m} M^{(a)} \,. \qquad (5)$$

Here *m* is the total number of microstates. Analyse how $< M >$ depends on *m*. In order words, calculate <M> after first 100 microstates (summation from m=1 to m=100) then after 200 microstates (summation from m=1 to m=200), then after 300 microstates (summation from m=1 to m=300), and so on (summation from m=1 to m=100xK). So you will get <M>(k) where k=1, ... K. Plot <M>(k) versus t=100 x k. It will show how <M> tends to the equilibrium value.

Parameters for simulations:
The number of spins: *N*=1000,
The number of generated microstates: *m*=100000,

The temperature range: T =[0.1, 10],
The temperature step: $\Delta T = 0.05$
Magnetic field: H =0.1.
Compare with the exact result:

$$M(T,H) = \frac{\sinh(\beta H)}{\sqrt{\sinh^2(\beta H) + e^{-4\beta J}}} \qquad (6)$$

Plot $M(T,H)$ as a function of T at a given H.

2. Ising model with all-to-all interaction (long-ranged interaction).

The energy of the Ising model with the long-ranged interaction is

$$E = -\frac{J}{N}\sum_{n=1}^{N-1}\sum_{m=n+1}^{N} S_n S_m - H\sum_{n=1}^{N} S_n\,, \qquad (9)$$

where $S_n = \pm 1$. The energy of spin S_n interacting with the other spins in a magnetic field H is

$$E_n(S_n) = -\frac{J}{N} S_n \sum_{m=1, m\neq n}^{N} S_m - HS_n \qquad (10)$$

One can choose J =1 as the energy unit.

Use the Metropolis algorithm and calculate the magnetization in the microstate a

$$M^{(a)} = \frac{1}{N}\sum_{n=1}^{N} S_n^{(a)}\,. \qquad (11)$$

Then, calculate the averaged magnetization and susceptibility:

$$< M > = \frac{1}{m}\sum_{a=1}^{m} M^{(a)}\,. \qquad (12)$$

$$\chi^{(a)} = \frac{N}{T}\left[\frac{1}{m}\sum_{a=1}^{m}(M^{(a)})^2 - < M >^2\right]. \qquad (13)$$

Here m is the total number of microstates. Compare the results of simulations with the exact results for M and χ given by the following equations:

$$M = \tanh\left[\beta J M + \beta H\right]\,, \qquad (14)$$

$$\chi = \frac{\beta}{\cosh^2\left[\beta J M + \beta H\right] - \beta J}\,. \qquad (15)$$

Plot M and χ versus T. Analyse a temperature dependence of M and χ near the critical point $T_c = J$.

Parameters for simulations:
The number of spins: N=100,
The number of generated microstates: m=50000,
The temperature range: T=[0.1, 10],
Magnetic field: H=0 or H=0.001
The temperature step: $\Delta T = 0.05$