Exercise 1. 3D Ising model

Goal: We continue simulating the Ising model by extending your code to work in three dimensions. We will use the Metropolis-based single-spin flip Monte Carlo method discussed in the lectures. As in Monte Carlo simulations the system size is limited whereas real physical systems are usually much larger, we can use Finite size scaling analysis technique to get good approximations for the thermodynamic limit (infinite system size).

Write a program for a Monte Carlo simulation to solve the three-dimensional Ising model with periodic boundary conditions. Implement the *single-spin flip* Metropolis algorithm for sampling.

If you are writing your code from scratch, note that you will have to reuse this code for upcoming exercise sheets and it might be worth to make sure that it is well-structured.

Task 1: Calculate the linear and nonlinear spin-spin correlation times τ and τ^{nl} for a few different temperatures using the correlation functions

$$\Phi_\sigma^{nl}(t) = \frac{\langle\sigma(t)\rangle - \langle\sigma(\infty)\rangle}{\langle\sigma(t_0)\rangle - \langle\sigma(\infty)\rangle} \sim \exp\left(-\frac{t}{\tau^{nl}}\right), \tag{1}$$

$$\Phi_\sigma(t) = \frac{\langle\sigma(t_0)\cdot\sigma(t)\rangle - \langle\sigma(t_0)\rangle^2}{\langle\sigma(t_0)^2\rangle - \langle\sigma(t_0)\rangle^2} \sim \exp\left(-\frac{t}{\tau}\right). \tag{2}$$

Use the results to determine how many update steps are needed to equilibrate the system, and how many updates need to be discarded between decorrelated samples. Also determine how this scheme changes close to the critical temperature.

Apply these results in your subsequents simulations.

Hint: Close to the critical temperature, you may use that $\nu \approx 0.63$ *and* $z \approx 2.09$.

Task 2: Measure and plot the *energy* E, the *magnetization* M, the *magnetic susceptibility* χ and the *heat capacity* C_V at different temperatures T.

Task 3: Determine the critical temperature T_c.

Hint: You should obtain $T_c \simeq 4.51$.

Task 4: Use your program to perform simulations of the Ising system for different system sizes to determine the critical exponents γ and ν for the magnetic susceptibility χ. Measure the temperature dependence of the susceptibility for different system sizes. Use the following formula for calculating the susceptibility (fluctuation-dissipation theorem):

$$\chi = N\beta\left(\langle M^2\rangle - \langle M\rangle^2\right)$$

where N is the number of spins, $\beta = 1/k_BT$ and M is the magnetization (magnetic moment per spin).

Task 5 (OPTIONAL): Vary γ/ν and $1/\nu$ until you get the best possible data collapse. The best way to judge the quality of the data collapse is by "eye". (Within the linear regions of the master curve the slope should be $-\gamma$. Check if the slope is correct as a verification of your data collapse.)

You might find the following points useful for solving Tasks 3 and 4:

- You can get an estimate for the ratio γ/ν by plotting the maximal value of χ depending on the system size (see lecture).
- Use that the critical temperature is given by $T_c \simeq 4.51$.
- You may try a more systematic way of determining the exponents:
  1. You can get an estimated value γ/ν as a start value. Try to get the best possible data collapse by tuning $1/\nu$ only.
  2. Within the linear regions of the master curve you can measure the slope $-\gamma$.
  3. Take the new values of γ and ν as new start value for γ/ν.