PHYS/ENGP 3170/6170
Computational Physics and Engineering
Spring 2021

Assignment #5: Thermodynamics of the Ising Model
Due: Mon, Apr 5 11:59 pm

Readings: LPB 17.1-17.4

The program Ising.py, provided with this assignment, implements the Metropolis algorithm for an Ising model of N=100 spins. The Hamiltonian is $E = - J \Sigma_j \, (s_j \, s_{j+1})$, where the spins s_j take values ±1 and the interaction constant J is set to +1 (ferromagnetic). Note that there is no external magnetic field. We also take k_B=1, i.e., temperature is measured in energy units. The temperature T is initially set to 100.0, which is much greater than J, so we are in the high-temperature regime. The program is set up to take a total of 200 steps, including accepted and rejected steps, after starting with an ordered configuration of all up spins.

(1) Modify the code to run for 1000 steps, and run the program to produce an output similar to Fig. 17.2, with "time" along the horizontal axis and position along the vertical axis.

(2) Plot the energy as a function of time for at least 1000 steps, and note approximately how long it takes to reach thermal equilibrium. Repeat with temperature T=1.0 (you may have to wait longer for equilibrium to be reached).

(3) You may want to switch to the Ising_faster.py version of the program, which only computes the change in the energy each time a spin is flipped instead of computing the energy from scratch. Extend the program to calculate the average energy $\langle E \rangle$ and average magnetization $\langle M \rangle$ (both defined in Eq. 17.14), over many steps, at temperature T=1.0. To get a non-zero average magnetization, you will need to add a small external magnetic field to the Hamiltonian: $E = - J \Sigma_j \, (s_j \, s_{j+1}) - B \, \Sigma_j \, s_j$, with B=0.001. Note that you should allow sufficient time for the system to thermally equilibrate before you begin averaging. Once the system has equilibrated, average over as many steps as you can to get reliable answers. Do your answers agree with the $N \to \infty$ predictions for the energy (Eq. 17.7, which assumes B=0) and the magnetization (Eq. 17.9)?

[Required for 6170 students only, extra credit for 3170 students] Also calculate the mean squared energy $\langle E^2 \rangle$, and thus the specific heat $C = (\langle E^2 \rangle - \langle E \rangle^2) / (N \, T^2)$ (see Eq. 15.18). Compare with the analytic prediction (Eq. 15.8).

(4) Measure the average energy and the average magnetization [and for 6170 students the specific heat] as functions of temperature, for $0 < T < 5$, and plot these along with the analytic expressions given on p. 413 (refer to Fig. 17.3 in the book for a rough idea of what your plots may look like). Use the same Hamiltonian as in the previous problem (J=1.0, B=0.001). To avoid having to re-equilibrate from scratch at every temperature,

use the following approach, inspired by simulated annealing: first equilibrate at T=5.0 for A steps and average over B steps, then reduce T to 4.9, equilibrate for A steps, and average over B steps at this new temperature, then reduce T to 4.8, etc. A needs to be large enough so that the cooling is slow and the system always remains in thermal equilibrium, while B needs to be large enough so that the averages you're measuring are not drowned out by statistical noise. You may need to play with these two parameters until you find values large enough to give stable results. State what values of A and B you end up using.