Physics 5403: Computational Physics – Project 8

---

due date: Dec 6, 2022

Monte-Carlo simulation of the square lattice Ising model

In this project you will perform a Monte-Carlo simulation of the Ising model, a simple model of a magnetic material. It consists of microscopic elementary magnets, the Ising spins S_i, on a square lattice. This spins can point up or down, represented by $S_i = \pm 1$. The energy of a particular spin configuration is given by

$$E = -J \sum_{\langle ij \rangle} S_i S_j \ .$$

The sum is over all pairs of nearest neighbor sites on the lattice. The interaction constant J is positive, so that the model favors parallel spins, i.e., ferromagnetism.

Your task is to simulate the behavior of this system using the Metropolis algorithm. The move class consists of single spin flips $S_i \to -S_i$, and the transition probability for such a flip is

$$W(S_i \to -S_i) = \begin{cases} \exp(-\Delta E/(k_B T)) & (\Delta E > 0) \\ 1 & (\Delta E < 0) \end{cases}$$

where ΔE is the change in total energy due to the spin flip and T is the temperature.

1. Write a program which performs the Monte-Carlo simulation of the Ising model on a square lattice of linear size L for several temperatures (you can work in units where $J = 1$ and $k_B = 1$). The program has to perform the following steps (i) set up the system (periodic or helical boundary conditions) and initialize the spins (hot and/or cold starts), (ii) perform a number of Monte-Carlo sweeps to equilibrate the system (a sweep is one attempted spin flip per lattice site). (iii) perform a number of Monte-Carlo sweeps to measure total energy, total magnetization, specific heat, and magnetic susceptibility.

2. Study the equilibration process by comparing runs with hot and cold starts for system size 50x50 and temperature T=2.5. Plot magnetization and energy as functions of Monte-Carlo time. Determine the necessary equilibration time for the following runs.

3. Perform measurements for a system of size 50x50 in the temperature interval $T = 1 \ldots 3$. Calculate magnetization, energy, susceptibility and specific heat as a function of temperature and make appropriate plots. Determine the approximate location of the phase transition.

4. Concentrate on the phase transition region and study the susceptibility and specific heat for varying system size (at least 20x20 to 500x500).

5. Determine the critical exponents α, β, and γ.