# MP468C — Computational Physics 2 — Lab 05

1. In assignment 5 you simulated the Ising chain

$$H \;=\; -\sum_{i=1}^{L-1} \sigma_i \sigma_{i+1} - B \sum_{i=1}^{L} \sigma_i \;.$$

   with **open** boundaries, i.e., the edge spins $i = 1$ and $i = L$ are only connected on one side.

   You might have treated these two sites specially in your code.

   Now consider the **periodic** Ising chain

$$H \;=\; -\sum_{i=1}^{L} \sigma_i \sigma_{i+1} - B \sum_{i=1}^{L} \sigma_i$$

   where the sum now includes a site $L+1$, which is identified with site 1. In other words, sites $L$ and 1 are now connected by Ising coupling.

   Modify your code to obtain the magnetization (per site) of this system. By using python's mod (%) operator, you might not have to treat the edge spins separately at all.

   For $L = 5$ and for $L = 20$, check if there is any noticeable difference between the magnetization calculated for the open chain and that calculated for the periodic chain. Use a temperature and a $B$ value of your choice.

2. Let's now consider the two-dimensional ferromagnetic Ising model

$$H \;=\; -\sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_{i} \sigma_i$$

   Take the lattice to be square-shaped, with $L_x \times L_y$ spins in total. The symbol $\langle ij \rangle$ indicates that the sites $i$ and $j$ are 'nearest neighbors'. Note that it is not easy to put explicit limits on the summations. Use periodic boundary conditions.

Write a function that generates a Markov chain, using the Metropolis algorithm.

Hint: first work out on paper what your accept/reject criterion is.

You could first use a $10 \times 10$ lattice. Increase this later if you can.

(a) Use your Markov chain first for temperature $T = 2$ (i.e., $\beta = 1/2$) and zero field $B = 0$. For these values, plot history curves for the energy and for the magnetization.

(b) Keeping the field at $B = 0$, vary temperature. Plot the average magnetization $\langle M \rangle$ as a function of temperature, ranging from $T = 4$ down to $T = 0.5$.

Plot the susceptibility $\chi$ as a function of temperature. If this curve has some interesting feature, zoom onto that temperature regime and calculate $\chi$ for a few more points in that regime.

3. Plan a MCMC calculation for calculating the autocorrelation function for the magnetization

$$R(t) = \langle M_n M_{n+t} \rangle - \langle M_n \rangle \langle M_{n+t} \rangle$$

where the subscripts indicate Monte Carlo step number, or Monte Carlo 'time'.

Code your strategy, calculate $R(t)$, and plot it as a function of $t$.

You might want to first attack the 1D chain, to be able to test in reasonable time.