MP468C — Computational Physics 2 — Lab 06

1. 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.

2. Consider the function

$$F(w) = \sum_{j=1}^{20} \left[wH(j/20) - G(j/20) \right]^2$$

with

$$H(x) = x^2 \qquad \text{and} \qquad G(x) = x^3 + 0.1\sin(30x)\,.$$

The function $F(w)$ is known to have a minimum between $w = -5$ and $w = +7$. Find this minimum using the method of golden sections.

3. Consider the one-dimensional ferromagnetic XY model. The 'spins' can now point in any direction within the x-y plane. The state of each spin is described by the angle $\theta_i \in [0, 2\pi)$ made with the x-axis.

$$H \;=\; -\sum_i \cos(\theta_i - \theta_{i+1}) - B \sum_i \cos(\theta_i)$$

There are L spins arranged linearly. You can use periodic or open boundary conditions, whichever you find easer — but make sure you treat the boundary spins correctly.

We want to generate a Markov chain. Previously (for Ising lattices), proposing moves involved flipping a spin, chosen at random. We can do something similar here, but what does 'flipping' a spin mean? θ_i has a continium of values $\in [0, 2\pi)$, not just two possible values. So, instead of flipping, I suggest proposing a new value of θ_i chosen uniform-randomly $\in [0, 2\pi)$.

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

Crucial hint: first work out on paper what your accept/reject criterion is. Do you need to calculate the total energies of the current state and proposed state?

Let's use this first for temperature $T = 2$ (i.e., $\beta = 1/2$) and zero field, $B = 0$.

You could first use a lattice (chain) size $L = 50$. Increase this later if you can.

(a) The magnetization now has x and y components!

$$M_x = \frac{1}{L} \sum_i \cos\theta_i \,, \qquad M_y = \frac{1}{L} \sum_i \sin\theta_i \,.$$

Draw history graphs for M_x, M_y and $M = \sqrt{M_x^2 + M_y^2}$.

(b) Plot the magnitude of the magnetization M as a function of temperature, for fixed $B = 0$.

(c) Plot the magnitude of the magnetization M as a function of field B, for fixed $T = 2$.