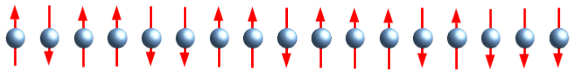

Exercise 11.1: Numerical simulation of the XY-model (6P)

Consider the one-dimensional classical XY model on a chain with L sites and closed boundary conditions (= no interaction between sites L und 1). Each lattice site $j = 1, \ldots, L$ is associated with a classical spin vector $s_j = \begin{pmatrix} \cos\theta_j \\ \sin\theta_j \end{pmatrix}$. The energy of a given configuration s reads

$$E_s \;=\; -J \sum_{<i,j>} s_i \cdot s_j - h \sum_j e_x \cdot s_j \;=\; -J \sum_{i=1}^{L-1} \cos(\theta_i - \theta_{i+1}) - h \sum_{j=1}^{L} \cos\theta_j \,.$$

In this model the partition sum is obtained by integrating over all angles:

$$Z(\beta) \;=\; \sum_{s \in \Omega_{sys}} e^{-\beta E_s} \;=\; \int_{-\pi}^{\pi} \mathrm{d}\theta_1 \int_{-\pi}^{\pi} \mathrm{d}\theta_2 \cdots \int_{-\pi}^{\pi} \mathrm{d}\theta_L \;\, e^{-\beta E(\theta_1,\ldots,\theta_L)}$$

(a) Show that for $h = 0$ the partition sum is given by $Z = 2\pi\big(2\pi I_0(\beta J)\big)^{L-1}$, where I_0 is the modified Bessel function of first kind. (2P)

(b) Read about the Ising Metropolis algorithm in the lecture notes and outline the Metropolis algorithm as an instruction sequence for the XY model. (2P)

(c) Prove that the Metropolis algorithm satisfies detailed balance in the stationary state. (2P)

Exercise 11.2: Method of stationary phase (6P)

Let us consider the following integral with an oscillating integrand

$$I(N) = \int_{-\infty}^{+\infty} f(t)\, e^{iN\psi(t)} \;\mathrm{d}t$$

with infinitely differentiable real-valued bounded smooth functions $\psi(t)$ and $f(t)$ in the limit of very large $N \in \mathbb{N}$.

(a) Give a qualitative explanation why for large N this integral will be dominated by the *stationary points* of the oscillating integrand where $\psi'(t) = 0$. (1P)

(b) Let $\epsilon > 0$ be small and fixed. Show that $\int_{T-\epsilon}^{T+\epsilon} f(t)\, e^{iN\psi(t)}\, \mathrm{d}t$ goes to zero as $N \to \infty$ provided that $\psi'(T) \neq 0$. What does it imply for $\lim_{N\to\infty} I(N)$ if $\psi(t)$ has no stationary points in the entire integration range? (2P)

(c) Suppose that the integrand has a single stationary point $\psi'(t) = 0$ at $t = T$. Compute the resulting contribution to $I(N)$ in the limit of very large N. You may use the identity $\int_{-\infty}^{+\infty} e^{i\alpha x^2}\, \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} e^{i\pi/4}$ for $\alpha > 0$. (3P)

(Σ = 12P)

To be submitted electronically on Wednesday, July 13, 2022, via WueCampus according to our guidelines on the web page `cs.hayehinrichsen.de`.