Sample Solutions Exercise 11

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)

Sample Solution

(a) Since we have closed boundary condition without an interaction between the last of the first site, it is possible to reorganize the integration. Only the first integral runs over the full range of θ_1 while the other ones run only over the difference angle $\Delta\theta_{i,i+1} = \theta_{i+1} - \theta_i$:

$$\int_{-\pi}^{\pi} \mathrm{d}\theta_1 \int_{-\pi}^{\pi} \mathrm{d}\theta_2 \cdots \int_{-\pi}^{\pi} \mathrm{d}\theta_L = \int_{-\pi}^{\pi} \mathrm{d}\theta_1 \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{12} \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{23} \cdots \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{L-1,L}$$

Since for $h = 0$ the partition sum $Z(\beta)$ depends only on the difference angles, the first integration over θ_1 is performed so to say without any effect and produces just a pre-factor 2π:

$$Z(\beta) = 2\pi \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{12} \cdots \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{L-1,L} \;\; e^{\beta J \sum_{i=1}^{L-1} \cos\Delta\theta_{i,i+1}}$$

The exponential function factorizes into:

$$Z(\beta) = 2\pi \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{12} \; e^{\beta J\cos\Delta\theta_{12}} \cdots \int_{-\pi}^{\pi} \mathrm{d}\Delta\theta_{L-1,L} \; e^{\beta J\cos\Delta\theta_{L-1,L}}$$

From $\int_{-\pi}^{+\pi} \mathrm{d}\theta \, e^{\beta J\cos\theta} = 2\pi I_0(\beta J)$ we arrive at the expression given in the exercise, which completes the proof.

(b) The update sequence of the Metropolis algorithm can be devised as follows:

- Randomly select a letter site i
- Store the angle θ_i and the current energy in temporary variables:

$$\theta_i^{old} := \theta_i \,, \qquad E_s^{old} := E_s$$

- Assign a new angle as a uniformly distributed random number $\theta_i := \mathrm{rand}(-\pi, +\pi)$.
- Calculate the new energy E_s and set $\Delta E := E_s - E_s^{old}$.
- If $\Delta E \leq 0$, then we accept the new angle and proceed with the next update.
- Otherwise, compute the probability $p = e^{-\beta\,\Delta E}$ and generate a uniformly distributed random number $z = \mathrm{rand}(0, 1)$.
- With probability p (i.e., if $z < p$) we accept the new angle and proceed with the next update.
- Otherwise we restore the old configuration by setting $\theta_i = \theta_i^{old}$.

Strictly speaking we would also have to verify that the proposed dynamics is ergodic, meaning that all configurations can be reached by the dynamic process. Obviously, this is indeed the case.

(c) We have to show that the Metropolis algorithm obeys the condition of detailed balance

$$\frac{p_{s'}^{stat}}{p_s^{stat}} = \frac{w_{s\to s'}}{w_{s'\to s}} \,.$$

The proof is largely independent of the specific model under consideration and works as follows (cf. lecture notes): We know that in the canonical ensemble the stationary state is given by $p_s^{stat} = \frac{1}{Z} e^{-\beta E_s}$, hence the left side of the equation above turns into

$$\frac{p_{s'}^{stat}}{p_s^{stat}} = e^{-\beta\,\Delta E_{s\to s'}} \,, \qquad \Delta E_{s\to s'} = E_{s'} - E_s \,.$$

Now we distinguish two different cases depending on the sign of $\Delta E_{s\to s'}$.

- If $\Delta E_{s\to s'} \leq 0$, then the transition in forward direction $s \to s'$ is executed at a rate $w_{s\to s'} = f$, where f is the update frequency of the algorithm. The rate for transition in opposite direction (for which the change in the energy would be positive) is less probable by the factor $e^{-\beta\,\Delta E}$, hence $w_{s'\to s} = f e^{+\beta\,\Delta E s\to s'}$. Consequently we have

$$\frac{w_{s\to s'}}{w_{s'\to s}} = \frac{f}{f e^{+\beta\,\Delta E s\to s'}} = e^{-\beta\,\Delta E s\to s'}$$

  confirming detailed balance.
- For the other case $\Delta E_{s\to s'} > 0$ the proof works in the same way; in this case $w_{s\to s'} = f e^{-\beta\,\Delta E_s}$ and $w_{s'\to s} = f$.

Exercise 11.2: Method of stationary phase (6P)

Let us consider the following integral with an oscillating integrand

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

in the limit of very large $N \in \mathbb{N}$. The two functions $\psi(t)$ and $f(t)$ and their derivatives are real-valued, smooth and bounded. Note that they do not depend on 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)

Sample Solution

(a) When N is large $f'(t) \neq 0$, the integrand will oscillate rapidly on the unit circle. Since $f(t)$ is smooth, we expect the contributions of the integrand to nearly cancel. This cancellation is expected to become increasingly effective when N is taken to infinity. However,in the vicinity of a stationary point $f'(t) = 0$ this cancellation mechanism is inhibited. This is where we expect to pick up dominant contributions. (1P)

(b) Solution by partial integration:
Approximating $\psi(t) \approx \psi(T) + \psi'(T)(t - T)$ we can integrate by parts: (2P)

$$\int_{T-\epsilon}^{T+\epsilon} f(t)\, e^{iN\psi(t)}\,\mathrm{d}t \;=\; \frac{f(t)}{iN\psi'(T)} e^{iN\psi(t)}\Big|_{T-\epsilon}^{T+\epsilon} - \frac{1}{iN\psi'(T)} \int_{T-\epsilon}^{T+\epsilon} f'(t)\, e^{iN\psi(t)}\,\mathrm{d}t\,.$$

Since both $f(t)$ and $f'(t)$ are bounded on the integration range, it is clear that both contributions on the r.h.s. scale like $1/N$, hence tend to zero in the limit $N \to \infty$.

Alternative solution by explicit integration:
Since ϵ is fixed and small, we can Taylor-expand both $f(t)$ and $\psi(t)$ to first order around T. This gives the following integral which can be carried out:

$$\int_{T-\epsilon}^{T+\epsilon} f(t)\, e^{iN\psi(t)}\,\mathrm{d}t \;=\; \int_{T-\epsilon}^{T+\epsilon} \Big(f(T) + f'(T)(t-T)\Big) e^{iN(\psi(T)+\psi'(T)(t-T))}\,\mathrm{d}t + \mathcal{O}(\epsilon^2)$$

$$= \frac{2if'(T)e^{i\mathrm{N}\psi(T)} \sin\left(\mathrm{N}\epsilon\psi'(T)\right)}{\mathrm{N}^2\psi'(T)^2} - \frac{2i\epsilon f'(T)e^{i\mathrm{N}\psi(T)} \cos\left(\mathrm{N}\epsilon\psi'(T)\right)}{\mathrm{N}\psi'(T)} + \frac{2f(T)e^{i\mathrm{N}\psi(T)} \sin\left(\mathrm{N}\epsilon\psi'(T)\right)}{\mathrm{N}\psi'(T)}$$

With the triangle relation we get: (1P)

$$\left|\int_{T-\epsilon}^{T+\epsilon} f(t)\, e^{iN\psi(t)}\,\mathrm{d}t\right| \;\leq\; \frac{2f'(T)}{N^2\psi'(T)^2} + \frac{2\epsilon f'(T)}{N\psi'(T)} + \frac{2f(T)}{N\psi'(T)}$$

This means that for fixed ϵ and $\psi'(T) \neq 0$ the contribution of this integral goes to zero like $1/N$ as $N \to \infty$. Consequently, if $\psi(t)$ has no stationary points in the entire integration range, and if we compose the full integration range into many small ones, we can conclude that (1P)

$$\lim_{N\to\infty} I(N) = 0.$$

Correction advice: There are subleties regarding uniform or non-uniform convergence to zero, which should be ignored in this exercise. This part can be solved in various ways. Important is the $1/N$-behavior and the final conclusion.

(c) Because of the result obtained in (b), the only contribution to $I(N)$ comes from the stationary point and its immediate vicinity. Hence for large N we have (1P)

$$I(N) \;\approx\; \int_{T-\epsilon}^{T+\epsilon} f(t)\, e^{iN\psi(t)} \;\simeq\; f(T) \int_{T-\epsilon}^{T+\epsilon} e^{iN\psi(t)}$$

Now we expand $\psi(t)$ to second order with $\psi'(T) = 0$: (1P)

$$\begin{aligned}
I(N) \;&\approx\; f(T) \int_{T-\epsilon}^{T+\epsilon} e^{iN\left(\psi(T)+\frac{1}{2}\psi''(T)(t-T)^2\right)} \,\mathrm{d}t \qquad \Big| \tau := t - T \\
&=\; f(T)\, e^{iN\psi(T)} \int_{-\epsilon}^{+\epsilon} e^{iN\frac{1}{2}\psi''(T)\tau^2} \,\mathrm{d}\tau \qquad \Big| x := \tau/\sqrt{N} \\
&=\; f(T)\, e^{iN\psi(T)} \frac{1}{\sqrt{N}} \int_{-\epsilon/N}^{+\epsilon/N} e^{i\frac{1}{2}\psi''(T)x^2} \,\mathrm{d}x \\
&\approx\; f(T)\, e^{iN\psi(T)} \frac{1}{\sqrt{N}} \int_{-\infty}^{+\infty} e^{i\frac{1}{2}\psi''(T)x^2} \,\mathrm{d}x
\end{aligned}$$

Now we can use the given integral to obtain (1P)

$$\boxed{I(N) \approx f(T)\, e^{iN\psi(T)\pm i\pi/4} \sqrt{\frac{2\pi}{N\,|\psi''(T)|}}}$$

(Σ = 12P)