Exercises for Computational Physics (physik760) WS 2017/2018

B. Kostrzewa, T. Luu, M. Petschlies and C. Urbach

1 Probability theory review

- 1: Show $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B) \mathbb{P}(AB)$.
- **2:** Show $\mathbb{P}(\bar{A}|B) = 1 \mathbb{P}(A|B)$.
- 3: $\mathbb{P}(A|\bar{B}) = (\mathbb{P}(A) \mathbb{P}(B)\mathbb{P}(A|B)) / (1 \mathbb{P}(B)).$

4: Let X, Y be **iid** normal distributed random variables (definition 2.2.5) with mean $\mu = 0$ and variance σ^2 . Show that Z = X + Y is a normal distributed random variable with mean $\mu = 0$ and variance $2\sigma^2$.

2 Simulation of the Ising model in two dimensions

The primary goal of simulating the model is to estimate physical observables. For the 2-dimensional Ising model these are defined as

$$\langle A \rangle = \sum_{s} P(s) A(s)$$
 (1)

$$P(s) = \frac{1}{N} \exp\left(-\frac{\mathcal{H}(s)}{k_B T}\right), \quad \mathcal{N} = \sum_{s'} \exp\left(-\frac{\mathcal{H}(s')}{k_B T}\right), \quad (2)$$

where we take A as a real-valued functional $A: s \mapsto \mathbb{R}$ on the space of spin configurations.

- 5: Identify the spin configurations of minimal and maximal energy, $H_{\min/\max}$. Can you find expressions for $H_{\min/\max}$ in terms if L_{σ} and L_{τ} ?
- **6:** Identify symmetries of the Hamiltonian and demonstrate them numerically by explicit application of the corresponding symmetry transformation.
- 7: For a given spin configuration s, the absolute value of the magnetisation per spin is an observable defined by

$$|m|(s) = \frac{1}{L_{\sigma} L_{\tau}} \left| \sum_{x \in \mathbb{L}} s_x \right|$$
 (3)

a) Implement the calculation of $\langle |m| \rangle$ using the weighted summation from eqs. (1), (2). Use units in which $k_B = 1$ and set J/T = 0.5.

- b) Compute $\langle |m| \rangle$ for $L_{\sigma} = L_{\tau} \in \{2, 3, 4, 5\}$. How long would your code take for the computation on a lattice with $L_{\sigma} = L_{\tau} = 10$ (100)?
- c) Run your code for $L_{\sigma}=L_{\tau}=10$, keep the (partial sum of) the absolute value of the magnetization every 200th configuration and plot the result.