Exercise 1. *Markov chains and invariant probability*

Let X be a finite state space and P be the transition matrix of a Markov chain on X. Suppose that P is reversible with respect to a probability measure π on X, i.e., it satisfies the "detailed balance" equation

$$\pi(x) P(x,y) = \pi(y) P(y,x) \text{ for all } x, y \in X.$$

Prove that the distribution is stationary for the Markov chain : let $(Y_n)_{n\in\mathbb{N}}$ be a Markov chain associated with P (i.e. $\mathbb{P}(Y_n = y_n | (Y_i)_{i=0}^{n-1} = (y_i)_{i=1}^{n-1}) = P(y_{n-1}, y_n)$), if the law of Y_0 is π then for any $n \in \mathbb{N}$, the law of Y_n is also π.

Exercise 2. *Low and high temperature of Ising model.*

Consider the Ising configurations $\sigma : \Omega \to \{-1, 1\}$ on a finite connected subset Ω of the square lattice $\mathbb{Z}^2$. This is the probability measure

$$\pi(\sigma) = \frac{1}{Z} e^{-\beta\mathcal{H}(\sigma)}$$

where $\mathcal{H}(\sigma) = -\sum_{i\sim j} \sigma_i\sigma_j$ and the partition function is given by $Z = Z(\beta) := \sum_\sigma e^{-\beta\mathcal{H}(\sigma)}$. What are the resulting measures on the state space $\{\pm 1\}^\Omega$ in the following limits?

1. $\beta \to 0$,
2. $\beta \to \infty$,
3. $\beta \to -\infty$ (the *anti-ferromagnetic limit*).

Hint : $e^{-\beta\mathcal{H}(\sigma)}$ penalizes configurations with high energy, i.e. with high $\mathcal{H}(\sigma)$. Also, notice how transformations of the form $\mathcal{H} \to \mathcal{H} + c$, where c is a constant, don't affect the measure : $\pi(\sigma) = \pi_{\mathcal{H}}(\sigma)$.

Exercise 3. *Observables computed using the partition function.*

The partition function $Z = Z(\beta)$ of the Ising model at inverse temperature β on a finite connected subset Ω_δ of the square lattice $\delta\mathbb{Z}^2$ can be exploited to calculate physical quantities in the model.

(1) Show that the average energy $\langle\mathcal{H}\rangle$ is given by:

$$\langle\mathcal{H}\rangle := \frac{1}{Z}\sum_\sigma \mathcal{H}(\sigma)\exp(-\beta\mathcal{H}(\sigma)) = -\frac{\partial}{\partial\beta}\ln Z.$$

(2) The entropy of a probability $(p(\sigma))_{\sigma:\Omega_\delta\to\{-1,1\}}$ is given by :

$$S := -\langle\ln(p)\rangle = -\mathbb{E}(\ln(p)) = -\sum_\sigma p(\sigma)\ln(p(\sigma)),$$

Show that for the Ising model, S_β is given by

$$S_\beta = \ln Z - \beta\frac{\partial}{\partial\beta}\ln Z = -\beta^2\frac{\partial}{\partial\beta}\left(\frac{1}{\beta}\ln Z\right).$$

(3) We can define the *free energy* as $\mathcal{F} = -T\ln Z$, with $T = \frac{1}{\beta}$ being the temperature of the system. Show that

$$S_\beta = -\frac{\partial\mathcal{F}}{\partial T}.$$

And that $\langle\mathcal{H}\rangle$, also called the *internal energy* of the system, is equal to :

$$\langle\mathcal{H}\rangle = \mathcal{F} + TS.$$

Remark. The former equation says that the total energy is split into two parts, the TS part, linked to the entropy of the system (quantifying how much it is disordered) and the second part $\mathcal{F}$, the *free energy*, which is the maximum amount of non-expansion work that can be extracted from the thermodynamically closed system at fixed temperature (and pressure).

(4) Let us now assume + boundary conditions and recall the GKS inequality

$$\langle\sigma_A\sigma_B\rangle_\beta^{\delta,+} \geq \langle\sigma_A\rangle_\beta^{\delta,+}\langle\sigma_B\rangle_\beta^{\delta,+}$$

where A, B are sets of vertices, and we used the notation $\mathbb{E}_{\Omega_\delta}^+[-] = \langle - \rangle_\beta^{\delta,+}$ and $\sigma_A = \prod_{x\in A}\sigma_x$. Using the GKS inequality, show that

$$\partial_\beta\mathbb{E}_{\Omega_\delta}^+[\sigma_A] \geq 0.$$