Exercise 1. 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.

Solution. Let us suppose that P is reversible with respect to a probability measure π on X. Then $\pi(x) P(x,y) = \pi(y) P(y,x)$ for all $x, y \in X$, and we can sum on x:

$$\sum_x \pi(x) P(x,y) = \sum_x \pi(y) P(y,x) = \pi(y)$$

since $\sum_x P(y,x) = 1$. Thus

$$\sum_x \pi(x) P(x,y) = \pi(y)$$

Let us remark that the left hand side is $\mathbb{P}(Y_1 = y)$ when the law of Y_0 is π and the right hand side is $\mathbb{P}(Y_0 = y)$. Thus we just proved that $\mathbb{P}(Y_1 = y) = \mathbb{P}(Y_0 = y)$ if f the law of Y_0 is π. By induction and using the Markov Property, we conclude that for any $n \in \mathbb{N}$, the law of Y_n is also π.

Exercise 2. 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 : $\pi(\sigma) = \pi_{\mathcal{H}}(\sigma)$.

Solution. Let us consider the different limiting regimes :

(1) $\beta \to 0$: in this case, for any σ, $e^{-\beta\mathcal{H}(\sigma)} \to 1$ and thus $Z \to 2^\Omega$. Therefore π converges to the uniform measure on the state space.

(2) $\beta \to +\infty$: this case is more tricky since $e^{-\beta\mathcal{H}(\sigma)} \to \mathbb{1}_{\mathcal{H}(\sigma)>0} \cdot 0 + \mathbb{1}_{\mathcal{H}(\sigma)<0} \cdot \infty + \mathbb{1}_{\mathcal{H}(\sigma)=0}$. Let us also remark that if there is any σ such that $\mathcal{H}(\sigma) < 0$ then $Z \to \infty$, whereas if all σ satisfy $\mathcal{H}(\sigma) > 0$ then $Z \to 0$. All this implies that one has to deal either with fractions like $\frac{0}{0}$ or $\frac{\infty}{\infty}$. Let us remark as well that if $\mathcal{H}(\sigma) \geq 0$ for all σ and there exist some configurations with 0 energy, then it is easy to see that the measure π converges to the uniform measure on the configurations of energy 0. It would therfore be nice if we could shift the energy by a constant, but this is possible ! Let us remark that if $\tilde{\mathcal{H}} = \mathcal{H} + c$ with $c = \mathbb{R}$, then

$$Z_{\tilde{\mathcal{H}}} = \sum_\sigma e^{-\beta\tilde{\mathcal{H}}(\sigma)} = \sum_\sigma e^{-\beta(\mathcal{H}(\sigma)+c)} = e^{-\beta c} Z_{\mathcal{H}}$$

and thus

$$\pi_{\tilde{\mathcal{H}}}(\sigma) := \frac{1}{Z_{\tilde{\mathcal{H}}}} e^{-\beta\tilde{\mathcal{H}}(\sigma)} = e^{-\beta\mathcal{H}(\sigma)} e^{-\beta c} e^{\beta c} \frac{1}{Z_{\mathcal{H}}} = \frac{1}{Z_{\mathcal{H}}} e^{-\beta\mathcal{H}(\sigma)} = \pi_{\mathcal{H}}(\sigma).$$

This proves that $\mathcal{H} + c$ defines the same probability on the configurations. Thus, we can consider, instead of $\mathcal{H}$, the hamiltonian $\mathcal{H} - \min_\sigma(\mathcal{H}(\sigma)) =: \tilde{\mathcal{H}}$ which satisfies that :

(a) for any configuration $\tilde{\mathcal{H}}(\sigma) \geq 0$,

(b) there exist configurations such that $\tilde{\mathcal{H}}(\sigma) = 0$, called the ground states, which are the two configurations such that $\sigma_x = 1$ or $\sigma_x = -1$ $\forall x$.

In particular, this proves that when $\beta \to +\infty$, the measure converges to the uniform measure on the two ground states.

(3) $\beta \to -\infty$: we can do a similar trick by considering $\mathcal{H} - \max_\sigma (\mathcal{H}(\sigma))$ and we can check that the measure converges to the uniform measure on the configurations with maximal energy which are those such that $x \sim y$ implies $\sigma_x \neq \sigma_y$ (there are again two such configurations)

Exercise 3. 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:

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

Solution. It is a simple computation :

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

(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

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

Solution. Let us compute the entropy:

$$S_\beta = -\sum_\sigma p(\sigma) \ln(p(\sigma)) = -\sum_\sigma \frac{e^{-\beta \mathcal{H}(\sigma)}}{Z} \ln\left(\frac{e^{-\beta \mathcal{H}(\sigma)}}{Z} \right)$$

hence

$$S_\beta = \beta \sum_\sigma \mathcal{H}(\sigma) \frac{e^{-\beta \mathcal{H}(\sigma)}}{Z} + \sum_\sigma \frac{e^{-\beta \mathcal{H}(\sigma)}}{Z} \ln(Z)$$

or using the fact that $Z = \sum_\sigma e^{-\beta \mathcal{H}(\sigma)}$, we get $S_\beta = \beta \langle \mathcal{H} \rangle + \ln(Z)$. Using the first question, this can be expressed as

$$S_\beta = \ln(Z) - \beta \frac{\partial}{\partial \beta} \ln Z.$$

A simple computation allow us to write

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

hence

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

(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).

Solution. Using the chain rule, since $\frac{\partial T}{\partial \beta} = -\frac{1}{\beta^2} = -T^2$, we get that

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

is equal to

$$S_\beta = -\frac{\partial}{\partial T}\left(-T\ln Z\right) = -\frac{\partial \mathcal{F}}{\partial T}.$$

hence the result. By expanding, we see that:

$$S_\beta = \ln Z + T\frac{\partial}{\partial T}\ln Z$$

hence

$$TS_\beta = -\mathcal{F} + T^2\frac{\partial}{\partial T}\ln Z.$$

Since $T^2\frac{\partial}{\partial T}\ln Z = -\partial_\beta \ln Z = \langle \mathcal{H}\rangle$ we get the formula:

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

(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

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

Solution. Let us first observe that

$$\frac{1}{Z}\sum_\sigma \mathcal{H}(\sigma)e^{-\beta\mathcal{H}(\sigma)} = -\frac{1}{Z}\sum_\sigma e^{-\beta\mathcal{H}(\sigma)}\sum_{x\sim y}\sigma_x\sigma_y = -\sum_{x\sim y}\langle \sigma_x\sigma_y\rangle_\beta^{\delta,+}.$$

Hence the result follows from the following computation, where the last inequality is a consequence of the GKS inequality:

$$\begin{aligned}
\partial_\beta \langle \sigma_A\rangle_\beta^{\delta,+} &= \partial_\beta\left(\frac{1}{Z}\sum_\sigma \sigma_A e^{-\beta\mathcal{H}(\sigma)}\right)\\
&= -\frac{\partial_\beta Z}{Z^2}\sum_\sigma \sigma_A e^{-\beta\mathcal{H}(\sigma)} - \frac{\beta}{Z}\sum_\sigma \sigma_A\mathcal{H}(\sigma)e^{-\beta\mathcal{H}(\sigma)}\\
&= \beta\frac{\sum_\sigma \mathcal{H}(\sigma)e^{-\beta\mathcal{H}(\sigma)}}{Z}\cdot\frac{\sum_\sigma \sigma_A e^{-\beta\mathcal{H}(\sigma)}}{Z} - \beta\frac{\sum_\sigma \sigma_A\mathcal{H}(\sigma)e^{-\beta\mathcal{H}(\sigma)}}{Z}\\
&= -\beta\sum_{x\sim y}\langle\sigma_x\sigma_y\rangle_\beta^{\delta,+}\langle\sigma_A\rangle_\beta^{\delta,+} + \beta\sum_{x\sim y}\langle\sigma_A\sigma_x\sigma_y\rangle_\beta^{\delta,+} = \beta\sum_{x\sim y}\left(\langle\sigma_A\sigma_x\sigma_y\rangle_\beta^{\delta,+} - \langle\sigma_x\sigma_y\rangle_\beta^{\delta,+}\langle\sigma_A\rangle_\beta^{\delta,+}\right) \geq 0.
\end{aligned}$$