

**Exercise 1. Rényi entropies**

One Schur-concave function you are already familiar with is the Shannon entropy. The Shannon entropy can be generalized to the Rényi entropies, defined for a vector of probabilities  $p$ :

$$S_\alpha(p) := -\frac{1}{\alpha - 1} \log \sum_{i=1}^m p_i^\alpha \quad (\alpha \in \mathbb{R}^+ \setminus \{0, 1\}),$$

with a few special cases corresponding to  $\alpha \in \{0, 1, \infty\}$ :

$$\begin{aligned} S_0(p) &:= \log \text{rank } p && (\text{max entropy}), \\ S_1(p) &:= -\sum_{i=1}^m p_i \log p_i && (\text{Shannon entropy}), \\ S_\infty(p) &:= -\log \max_i p_i && (\text{min entropy}). \end{aligned}$$

Show that:

- (a) The definitions of three special cases are consistent with the general formula:

$$\begin{aligned} \lim_{\alpha \rightarrow 0} S_\alpha &= S_0, \\ \lim_{\alpha \rightarrow 1} S_\alpha &= S_1, \\ \lim_{\alpha \rightarrow \infty} S_\alpha &= S_\infty. \end{aligned}$$

- (b) All Rényi entropies are Schur-concave.  
(c) All Rényi entropies have values between 0 (for a pure distribution) and  $\log n$  (for a maximally mixed distribution), where  $n$  is the size of the system.

Now let us define the relative Rényi entropies as

$$S_\alpha(p||q) := \frac{\text{sgn}(\alpha)}{\alpha - 1} \log \sum_{i=1}^m p_i^\alpha q_i^{1-\alpha} \quad (\alpha \in \mathbb{R} \setminus \{1\}),$$

where we set  $0^0 := 0$ , and  $\text{sgn}(\alpha) = \begin{cases} +1 & \text{if } \alpha \in [0, +\infty] \\ -1 & \text{if } \alpha \in [-\infty, 0). \end{cases}$

- (d) Show that  $\lim_{\alpha \rightarrow 1} S_\alpha(p||q) = S(p||q)$ , where  $S(p||q)$  is the usual conditional entropy,  $S(p||q) = \sum_{i=1}^m p_i \log \frac{p_i}{q_i}$ .

## Exercise 2. Thermal operations with restrictions

One of the important quantities at macroscopic scale is (Helmholz) free energy:

$$F(\rho) = E(\rho) - TS(\rho).$$

At constant ambient temperature  $T$  and constant volume, transitions between two states are possible if and only if the difference between the free energies of the initial and the final states is negative. This free-energy difference also tells us how much work we can extract, or need to invest, during a thermodynamic state transition.

At the microscopic scale, however, the possibility of state transitions is not determined by free energy alone, but by an infinite family of free-energy-like quantities. These known results rely crucially on the assumption that the thermal machine is not only exactly preserved in every cycle but also kept uncorrelated from the quantum systems on which it acts:

$$\rho_A \otimes \sigma_M \mapsto \rho'_A \otimes \sigma_M$$

We assume that the machine can strictly only perform the following operations: energy-preserving unitaries; accessing thermal states from the bath; and ignoring heat bath degrees of freedom by tracing over them (thermal operations). If we assume for the moment that there is no work reservoir  $W$ , and demand that these operations preserve the local state of the machine  $M$  and also its independence from  $A$ , then they describe transitions  $\rho_A \rightarrow \rho'_A$ . It has been shown [1] that a thermal transformation can achieve this transition (up to an arbitrarily small error on  $A$ ) if and only if all  $\alpha$ -free energies decrease in the process:

$$\Delta F_\alpha = F_\alpha(\rho'_A) - F_\alpha(\rho_A) \leq 0 \text{ for all } \alpha \geq 0. \quad (1)$$

Here  $F_\alpha(\rho_A) = k_B T S_\alpha(\rho_A || \gamma_A) - k_B T \log Z_A$ , with  $Z_A$  the partition function of  $A$ ,  $T$  the background temperature,  $k_B$  Boltzmann's constant, and  $S_\alpha$  the Rényi divergence of order  $\alpha$  (see previous exercise). For  $\alpha \in \{-\infty, 0, 1, \infty\}$ , we use the definitions

$$S_0(p||q) = \lim_{\alpha \searrow 0} S_\alpha(p||q) = -\log \sum_{i:p_i \neq 0} q_i, \quad S_1(p||q) \equiv S(p||q),$$

$$S_\infty(p||q) = \lim_{\alpha \rightarrow \infty} S_\alpha(p||q) = \log \max_i \frac{p_i}{q_i}, \quad S_{-\infty}(p||q) = \lim_{\alpha \rightarrow -\infty} S_\alpha(p||q) = S_\infty(q||p).$$

- (a) For  $\alpha = 1$ , show that the free energy reduces to the Helmholtz free energy  $F_1 = F$ .

Here, we look at general transformations of the form:

$$\rho_A \otimes \sigma_M \mapsto \sigma_{AM}, \text{ with } \text{tr}_M(\sigma_{MA}) = \rho'_A \text{ and } \text{tr}_A(\sigma_{MA}) = \sigma_M.$$

To see that the  $\alpha$ -free energies impose severe constraints on the workings of a thermal machine, let us look at a simple example.

- (b) Suppose that a thermal machine is supposed to heat up a system  $A$  from its thermal state  $\gamma_A$  to infinite temperature (a fully mixed state). Suppose that  $A$  is a qubit with energies 0 and  $E_A$ , its initial temperature is such that  $\beta E_A = \log 2$ . The associated work cost will

be delivered by an additional work bit  $W$  with energy gap  $\Delta > 0$ . It starts in its excited state  $|e\rangle$  and will end up in its ground state  $|g\rangle$ . The machine implements the transition

$$\gamma_A \otimes |e\rangle\langle e|_W \mapsto \rho'_A \otimes |g\rangle\langle g|_W$$

with a work cost  $\Delta$  that is as small as possible. As before, this is achieved by a catalytic thermal operation of the form

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \mapsto \rho'_A \otimes \sigma_M \otimes |g\rangle\langle g|_W$$

Calculate the  $\alpha$ -energy difference for  $\alpha \rightarrow \infty$ . For which work bit gaps  $\Delta$  is this difference  $\leq 0$  for all  $\alpha$ ? Compare this case to the usual free energy difference ( $\alpha = 1$ ).

One reason for the discrepancy is that we are dealing with the case of a single system only. Intuitively, by acting collectively on a large number of particles, a machine can achieve more than if it had to act on each particle separately.

We thus have two independent motivations to allow correlations between  $M$  and  $AW$ : the difficulty to avoid correlations on interaction, and the desire to achieve higher efficiency. We will now show that the latter goal can indeed be achieved by allowing correlations to build up, *even if the catalyst  $M$  is as small as a single qubit*.

Let us now enforce thermal transitions of the form

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \longrightarrow \rho'_{AM} \otimes |g\rangle\langle g|_W,$$

- (c) Suppose that  $M$  has a trivial Hamiltonian,  $H_M = 0$ , and two basis states  $|0\rangle$  and  $|1\rangle$  (both of energy zero). Denote ground and excited state of  $A$  by  $|g_A\rangle$  and  $|e_A\rangle$ . Consider a correlated state of  $A$  and  $M$

$$\begin{aligned} \rho'_{AM} &:= \frac{1}{10}|g_A0\rangle\langle g_A0| + \frac{4}{10}|g_A1\rangle\langle g_A1| \\ &\quad + \frac{2}{10}|e_A0\rangle\langle e_A0| + \frac{3}{10}|e_A1\rangle\langle e_A1|. \end{aligned}$$

What are the reduced states of  $A$  ( $\rho'_A$ ) and  $M$  ( $\sigma_M$ )?

- (d) Now enforce the thermal transition of a form

$$\gamma_A \otimes \sigma_M \otimes |e\rangle\langle e|_W \longrightarrow \rho'_{AM} \otimes |g\rangle\langle g|_W.$$

How much work do we need to spend on this process? Compare with the value given by assuming a catalytic transition.

*Hint: Use Lorenz curves. You can take advantage of Matlab or Mathematica, too.*

It can be shown that only the standard Helmholtz free energy condition  $\Delta F_1 \equiv \Delta F \leq 0$  survives as a relevant necessary condition for a correlating state transition. For details, please consult [2].

## References

- [1] F. Brandão, M. Horodecki, N. Ng, J. Oppenheim, and S. Wehner, *The Second Laws of Quantum Thermodynamics*. **Proc. Natl. Acad. Sci. U.S.A.** **112**, 3275 (2015).  
 [2] Markus P. Müller, *Correlating Thermal Machines and the Second Law at the Nanoscale*. **Physical Review X**, **8**(4) (2018).