Exercise set 3

AI

1 Time derivative of the Kullback–Leibler divergence

The Kullback–Leibler divergence (or entropy) is a measure of dissimilarity between two probability distributions $\boldsymbol{P}$, $\boldsymbol{Q}$ and is defined as

$$D_{\mathrm{KL}}(\boldsymbol{P}, \boldsymbol{Q}) = \sum_x P(x) \log \frac{P(x)}{Q(x)}. \tag{1}$$

It can be shown that $D_{\mathrm{KL}}(\boldsymbol{P}, \boldsymbol{Q}) \geq 0$ with the equality holding only if $P(x) = Q(x),\ \forall x$.

Let $\boldsymbol{P}(t)$ be the solution of a master equation with time-independent rates $k_{x,x'}$ that satisfy the equilibrium detailed balance condition

$$k_{xx'}/k_{x'x} = \exp\left[-\beta(\epsilon_x - \epsilon_{x'})\right]. \tag{2}$$

Consider the KL divergence $D_{\mathrm{KL}}(\boldsymbol{P}(t), \boldsymbol{P}^{eq})$ and show that

$$\frac{\mathrm{d}}{\mathrm{d}t} D_{\mathrm{KL}}(\boldsymbol{P}(t), \boldsymbol{P}^{eq}) \leq 0,\ \forall t. \tag{3}$$

Hints: find a relation between the KL divergence in eq. (3) and the entropy production rate for the same process

$$\left\langle \dot{s}^{tot} \right\rangle. \tag{4}$$

You can either consider the entropy variation in the system and in the bath, or retrace the steps that lead to the Schnakenberg formula for entropy production.

2 Jarzynski equality for a sudden manipulation

A system with Hamiltonian $H_0(x)$ is at equilibrium at temperature T for $t < 0$.

At $t = 0$ the Hamiltonian is suddenly changed to $H_1(x)$ (a quench). You can imagine, for example, a sudden change in the external magnetic field in the Ising Hamiltonian.

Prove the Jarzynski equality for such a manipulation

$$\left\langle \mathrm{e}^{-\beta W} \right\rangle = \mathrm{e}^{-\beta \Delta F}$$

3 Work distribution in a quench

A particle is in contact with an environment at temperature T and moves in a potential

$$U(x) = \frac{k}{2} x^2. \tag{5}$$

Evaluate the probability density $p_F(w)$ of the work performed when the potential strength k is suddenly changed from k_0 to k_f, assuming that the particle is initially in thermal equilibrium with the strength k_0. Evaluate also the corresponding distribution $p_R(w)$ for the reverse process, assuming that the particle is initially at equilibrium with the strength k_f. Verify the detailed fluctuation relation

$$\frac{p_F(w)}{p_R(-w)} = \exp\left[\beta(w - \Delta F)\right], \tag{6}$$

with $\Delta F = F_f - F_0$.

Show that the distributions exhibit exponential tails.

4 Dragged particle in one dimension

Consider the dragged particle previously introduced in class moving on a ring lattice with rates p and q (or k_+ and k_-)$\cdot$ Show that the probability distribution of the total entropy s^{tot} produced in a time interval (t_0, t_f) satisfies the detailed fluctuation theorem. Assume that the system is already in the steady state at t_0.