

3.1. One assumes

$$\langle \delta(x - x_t) e^{-\beta W(t)} \rangle = \frac{e^{-\beta H(x, \lambda_t)}}{Z_0}$$

Integrate over x and choose t to be final time, then:

$$\langle e^{-\beta W} \rangle = \frac{1}{Z_0} \int e^{-\beta H(x, \lambda_t)} dx = \frac{Z_{\lambda_t}}{Z_0} = e^{-\beta \Delta F}$$

3.2 $\langle \delta(x - x_t) e^{-\beta W(t)} \rangle = \langle e^{-\beta W(t)} | x = x_t \rangle \underbrace{\langle \delta(x - x_t) \rangle}_{\rho(x, t)}$

$$= \frac{e^{-\beta H(x, \lambda_t)}}{Z_0}$$

Now dividing by $\rho_{eq}(x, \lambda_t) = \frac{e^{-\beta H(x, \lambda_t)}}{Z_t}$, one obtains

$$\frac{\rho(x, t)}{\rho_{eq}(x, \lambda_t)} \langle e^{-\beta W(t)} | x = x_t \rangle = \frac{e^{-\beta H(x, \lambda_t)}}{Z_0} \frac{Z_t}{e^{-\beta H(x, \lambda_t)}} = e^{-\beta \Delta F(t)}$$

where $\Delta F(t) = F_{\lambda_t} - F_{\lambda_0}$ is the free energy difference between a state with a control parameter λ_t and a state with a control parameter λ_0 .

Rq it is important to appreciate that at time t , the system may not be in equilibrium although the equilibrium free energy shows up in Jarzynski relation and is evaluated at $\lambda = \lambda_t$.

3.3 The free energy F and internal energy U are state functions, therefore their variation on a cycle is zero

$$\Delta F = \Delta U = 0$$

3.4 One can use the previous relation evaluated at the end of the protocol $t = \tau$:

$$\langle e^{-\beta W} \rangle_{x=x_c} = \frac{p_{eq}(x, \tau)}{p(x, \tau)}$$

If one considers only trajectories ending in the right minimum at time τ , then $p(x=x_R, \tau) = 1$ and $p_{eq}(x, \tau) = \frac{1}{2}$ given the initial condition (left or right with equal proba)

Thus $\langle e^{-\beta W} \rangle_{\rightarrow 0} = \frac{1}{2}$

Similarly one gets $\langle e^{-\beta W} \rangle_{\rightarrow 1} = \frac{1}{2}$

3.5 If the process is not perfect, we have instead

$p(x=x_R, \tau) = P_s$, then

$$\langle e^{-\beta W} \rangle_{\rightarrow 0} = \frac{1}{2P_s} \quad \text{and} \quad \langle e^{-\beta W} \rangle_{\rightarrow 1} = \frac{1}{2(1-P_s)}$$

Then taken together, the usual Jarzynski relation is recovered

$$\begin{aligned} \langle e^{-\beta W} \rangle &= P_s \langle e^{-\beta W} \rangle_{\rightarrow 0} + (1-P_s) \langle e^{-\beta W} \rangle_{\rightarrow 1} \\ &= \frac{1}{2} + \frac{1}{2} = 1. \end{aligned}$$

3.6 Using Jensen's inequality $\langle e^x \rangle \geq e^{\langle x \rangle}$, one obtains

$$\beta \langle W \rangle \geq \ln 2 + P_s \ln P_s + (1-P_s) \ln(1-P_s)$$

Using general expression of Shannon entropy $S = -k \sum_i p_i \ln p_i$

for a probability distribution p_i , it follows that

$$S_{t=0} = -k \left(\frac{1}{2} \ln \frac{1}{2} + \frac{1}{2} \ln \frac{1}{2} \right) = k \ln 2$$

$$S_{t=\tau} = -k (P_s \ln P_s + (1-P_s) \ln(1-P_s))$$

thus $\Delta S = k [\ln 2 + P_s \ln P_s + (1-P_s) \ln(1-P_s)]$

and $\beta \langle W \rangle \geq \frac{\Delta S}{k}$

or $\langle W \rangle \geq T \Delta S$

3.7 The figure shows that in the quasi-static limit

$$\zeta \rightarrow 0, \quad \langle Q \rangle \rightarrow kT \ln 2$$

Since $\langle \Delta U \rangle = 0 = \langle W \rangle - \langle Q \rangle$, this means

$\langle W \rangle \rightarrow kT \ln 2$ which corresponds to the expected result when $P_s \rightarrow 1$.

The process corresponds to a logically irreversible operation because the output (a particle always in the right well) does not permit to predict the input (a particle in the right or left).