©

Second law and (sub) systems
A simplified framework.

cf Jarzynski, PRL, 1996.

0

Setting:
We here describe a simplified framework to discuss the second law in the framework of thermalized systems.

- Consider a subsystem (Σ)

  (i) In contact with a thermal bath at inverse temperature $\beta = \frac{1}{k}$

  (ii) Described by a time-dependent Hamiltonian:

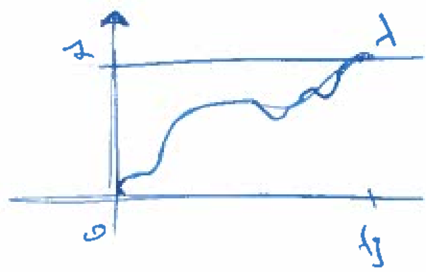
$$H[q, p, \lambda(t)].$$

"protocol"

  (iii) Driven by an external protocol. λ (smooth).

For simplicity, $\lambda : \mathbb{R} \to [0,1]$;

such that
$$\begin{cases} \lambda(t) = 0 & t < 0 . \\ \lambda(t) = 1 & t > t_f \quad \text{for some } t_f > \end{cases}$$



  (iv) Disconnected from the bath between $t=0$ and $t = t_f$.

  (v) At equilibrium at $t = -\infty$ and $t = +\infty$:

$$\rho_0 = \rho(t \to -\infty, p, q) = \exp - \beta H_0 + \beta F_0 . \qquad H_0 \doteq H(t=0)$$

$$\rho_F = \rho(t \to \infty, p, q) = \exp - \beta H_f + \beta F_f \qquad H_f = H(t = t_f).$$

Exercises:

① Show the first law of thermodynamics:

$$E_f - E_0 = \overline{W} + Q.$$

with

$$E_f = \langle H_f \rangle_f . \qquad \langle \cdot \rangle_f = \int d\vec{p}\, d\hat{q}\, e^{-\beta H_f + \dots}$$

$$E_0 = \langle H_0 \rangle_0 .$$

$$\overline{W} = \int_0^{t_f} \left\langle \dot{\lambda} \frac{\partial H}{\partial \lambda} \right\rangle_0 . \longrightarrow \text{Justify definition!}$$

$$Q = \langle H_f \rangle_f - \langle H_f \rangle_0 .$$

② Show the Jarzynski equality:

$$\left\langle e^{-\beta W} \right\rangle_0 = e^{-\beta \Delta F} \qquad \Delta F = F_f - F_0 .$$

③ Show the second law:

$$(*) \quad \Delta F \leqslant \langle W \rangle_0 . \qquad W = \int_0^{t_f} \dot{\lambda} \frac{\partial H}{\partial \lambda} .$$

- Justify the name "free energy" for ΔF.

④ Define the Boltzmann entropies $S_{0/f} = k_B \log W(E_{0/f})$. to justify that (*) indeed implies a positive entropy creation between $-\infty$ and ∞

$$S_{crea} \doteq \Delta S - \frac{Q}{T} \geqslant 0 .$$