ENTROPIES AND FLUCTUATIONS IN NON-EQUILIBRIUM SYSTEMS

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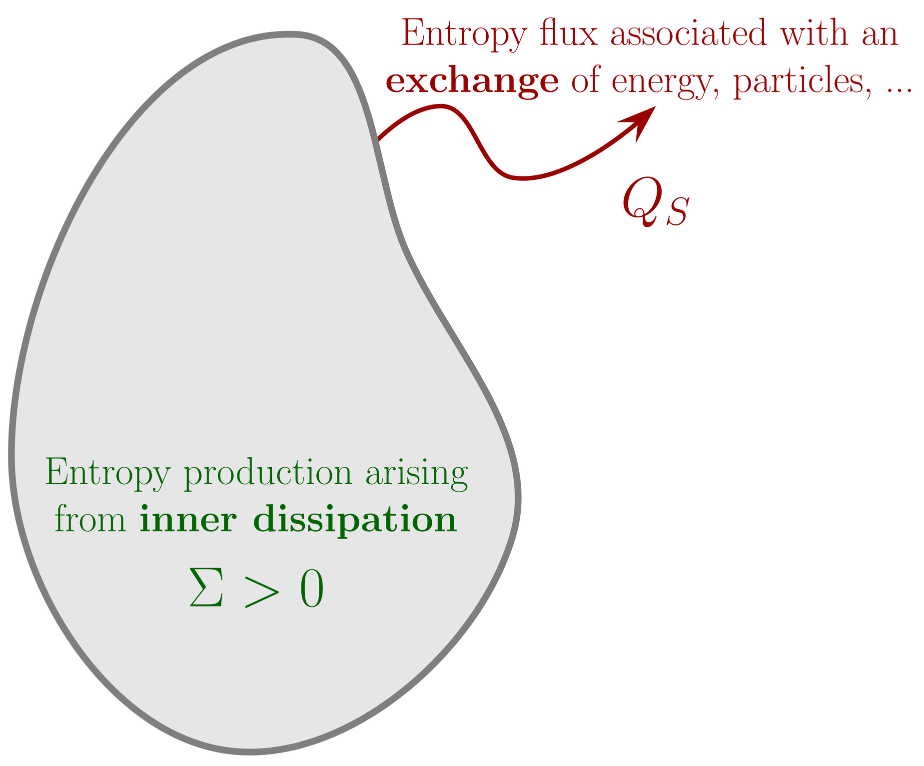
Abstract

The 19$^{\text{th}}$ century macroscopic equilibrium thermodynamics can be understood from a microscopic point of view through the statistical approach of Boltzmann and Gibbs. The general study of non-equilibrium states proves however more difficult and shows remarkably different features. We studied how different notions of entropy can be linked and give insights into the characteristics of fluctuations in such systems.

Entropy in macroscopic thermodynamics



- Macroscopic entropy balance (**time-averaged** quantities):

$$\text{Entropy Variation} \quad = \quad \underbrace{\text{Entropy Production}}_{>0} \quad - \quad \text{Entropy Exchange}$$

- Time reversibility:

$$\text{Equilibrium} \quad \Leftrightarrow \quad \text{Entropy Production} = 0$$

- Some common examples:

$$\text{Entropy Exchange} \quad = \quad \begin{cases} \frac{1}{T}\,\Delta Q & \text{(contact with a thermostat)} \\ \frac{1}{T}\,\mu\,\Delta N & \text{(c. with a particle reservoir)} \end{cases}$$

Question: can we find a microscopic point of view ?
→ systems with stochastic dynamics
→ entropy exchange seen as ⟨ history-dependent entropy exchange ⟩

The Lebowitz-Spohn-Gaspard-Maes approach

System with Markovian dynamics among its configurations $\{\mathcal{C}\}$:

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big[W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',t) - W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},t) \Big]$$

- The integrated entropy flow for an history $\mathcal{C}_0 \to \ldots \to \mathcal{C}_n$:

$$Q_S = \log \frac{W(\mathcal{C}_0 \to \mathcal{C}_1) \ldots W(\mathcal{C}_{n-1} \to \mathcal{C}_n)}{W(\mathcal{C}_0 \leftarrow \mathcal{C}_1) \ldots W(\mathcal{C}_{n-1} \leftarrow \mathcal{C}_n)}$$

is compatible with the variation of the Gibbs entropy $S_G = -\sum_{\mathcal{C}} P(\mathcal{C},t) \log P(\mathcal{C},t)$:

$$S_G(t) - S_G(0) = \underbrace{\Sigma(t)}_{>0} - \langle Q_S(t) \rangle$$

- In equilibrium (stationary state with detailed balance): $Q_S = 0$ and thus $\Sigma(t) = 0$.
- Fluctuation theorem:

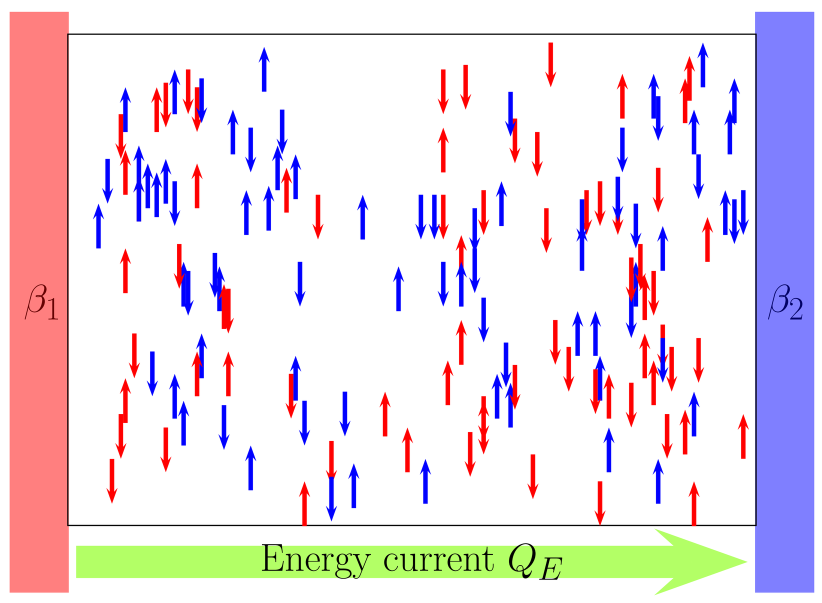
$$\text{Defining} \quad \langle e^{-s\,Q_S(t)} \rangle \sim e^{t\,\mu(s)} \quad \text{one has} \quad \mu(s) = \mu(1-s)$$

or equivalently

$$\text{Defining} \quad P\big(Q_S(t)/t = j_S\big) \sim e^{t\,\pi(j_S)} \quad \text{one has} \quad \pi(j_S) = j_S + \pi(-j_S)$$

Question: can we link $Q_S(t)$ to other quantities ?

Entropy flow distribution in a two-temperature Ising model [1]



N Ising spins σ_i on a complete graph interacting with two thermal baths at inverse temperature β_1 and β_2.

- Transition rates are:

$$W(\sigma_i \to -\sigma_i) = \begin{cases} e^{-\beta_1 \sum_i \sigma_i / N} & \text{if} \quad \sigma_i \in \mathbf{1} \\ e^{-\beta_2 \sum_i \sigma_i / N} & \text{if} \quad \sigma_i \in \mathbf{2} \end{cases}$$

- Non-equilibrium stationary state:

$$\text{Entropy Production} \quad = \quad \text{Entropy Exchange}$$

- Energy conservation:

$$\text{Energy current (System} \to \mathbf{1}\text{)} = -\text{Energy current (System} \to \mathbf{2}\text{)} \equiv Q_E$$

- Entropy exchange:

$$Q_S \quad = \quad \beta_1 Q_{E\mathbf{1}} + \beta_2 Q_{E\mathbf{2}} \quad = \quad (\beta_1 - \beta_2)\, Q_E$$

- The large deviation function of the entropy/energy current of this highly out-of-equilibrium system can be computed exactly:

$$\pi(j) = \tfrac{1}{2}\varepsilon\, j + 2 - \beta - \frac{1}{2}\sqrt{(2-\beta) + \varepsilon^2}\sqrt{4 + j^2} \quad \text{with} \quad \beta_{1,2} = \beta \pm \varepsilon$$

Link with the Kolmogorov-Sinai entropy of stochastic systems [2]

A central quantity in dynamical system theory: the *dynamical partition function*

$$Z(s,t) = \sum_{\substack{\text{histories} \\ \text{from } 0 \to t}} \big(\text{Prob}\{\text{history}\}\big)^{1-s}$$

- Topological pressure: $\psi(s) = \lim_{t\to\infty} \log Z(s,t)$
- Kolmogorov-Sinai entropy:

$$h_{\text{KS}} = -\frac{1}{t} \sum_{\text{hist.}} \text{Prob}\{\text{history}\} \ln \text{Prob}\{\text{history}\} = \psi'(0)$$

- Generalization to stochastic systems:
  − discrete time dynamics is OK (Gaspard *et al*)
  − sending the time step to zero is problematic
- A direct **continuous-time dynamics** approach enables to understand $Z(s,t)$ as the generating function of the momenta of an observable Q_+:

$$Z(s,t) = \langle e^{-s\,Q_+(t)} \rangle$$

with

$$Q_\pm(t) = \sum_{k=0}^{n-1} \ln \frac{W(\mathcal{C}_k \rightleftarrows \mathcal{C}_{k+1})}{r(\mathcal{C}_k)} \quad \text{and} \quad r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C} \to \mathcal{C}')$$

- The topological pressure $\psi(s)$ appears as the largest eigenvalue of the operator:

$$\mathbb{W}_+(\mathcal{C},\mathcal{C}') = W(\mathcal{C}' \to \mathcal{C})^{1-s} r(\mathcal{C}')^s - r(\mathcal{C})\delta_{\mathcal{C},\mathcal{C}'}$$

- Kolmogorov-Sinai entropy:

$$h_{\text{KS}} \; = \; -\left\langle \sum_{\mathcal{C}'} W(\mathcal{C} \to \mathcal{C}') \ln \frac{W(\mathcal{C} \to \mathcal{C}')}{r(\mathcal{C})} \right\rangle \; = \; -\frac{\langle Q_+ \rangle}{t}$$

- For the time-reversed trajectories: $h^R_{\text{KS}} = -\frac{\langle Q_- \rangle}{t}$
- Link between (history-dependent) integrated currents: $Q_S(t) \; = \; Q_+(t) - Q_-(t)$
- Link with the Kolmogorov-Sinai entropy: $j_S \; = \; h^R_{\text{KS}} - h_{\text{KS}}$
- The topological pressure can be computed in many equilibrium or non-equilibrium Markov systems.

References

[1] Vivien Lecomte, Zoltán Rácz and Frédéric van Wijland, *Energy flux distribution in a two-temperature Ising model* J. Stat. Mech. P02008 (2005) `[cond-mat/0412547]`

[2] Vivien Lecomte, Cécile Appert-Rolland and Frédéric van Wijland, *Chaotic Properties of Systems with Markov Dynamics* Phys. Rev. Lett. 95, 010601 (2005) `[cond-mat/0505483]`