Thermodynamic entropy production: Measure of quantum frameness

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Contents

Von Neumann S vs thermodynamic $S^{\rm th}$ entropies

Homogeneous equilibrium reservoir at temperature $k_B T = 1/\beta$ and volume V, with Hamiltonian H:

$$\rho_\beta = Z_\beta^{-1} \mathrm{e}^{-\beta H} \ .$$

Von Neumann (microscopic) entropy:

$$S(\rho_\beta) =: -\mathrm{tr}(\rho_\beta \log \rho_\beta)$$

coincides with the thermodynamic (macroscopic) entropy $S^{\rm th}$ in the thermodynamic limit $V \to \infty$.
For non-equilibrium: general proof is missing. Let's enforces the coincidence of von Neumann and thermodynamic entropy productions.
Issue: ΔS is zero as long as $\rho_\beta \to U \rho_\beta U^\dagger$, while $\Delta S^{\rm th} > 0$.
Solution: a 'graceful' irreversible map

$$\rho \to \mathcal{M} \rho$$

constrained by

$$\Delta S =: S(\mathcal{M} U \rho_\beta U^\dagger) - S(\rho_\beta) = \Delta S^{\rm th}.$$

Key quantity will be the *relative q-entropy*:

$$S(\sigma|\rho) =: \mathrm{tr}[\sigma(\log \sigma - \log \rho)] \ .$$

S and $S^{\rm th}$ in non-equilibrium

Apply an external field, limited in space and time:

$$\rho_\beta \to \rho'_\beta = U\rho_\beta U^\dagger \ .$$

To engineer von Neumann entropy production, we assume an irreversible map $\mathcal{M}$ to be specified later:

$$\Delta S =: S(\mathcal{M}\rho'_\beta) - S(\rho_\beta) \ > 0 \ .$$

To make it equal with $\Delta S^{\rm th}$, we need $\Delta S^{\rm th}$'s microscopic expression! The field performs work:

$$W =: {\rm tr}(H\rho'_\beta) - {\rm tr}(H\rho_\beta) = {\rm tr}[(\rho'_\beta - \rho_\beta)H] \ .$$

From ρ_β, express $H = -\beta^{-1}\log(Z_\beta\rho_\beta)$, and consider $\rho'_\beta = U\rho_\beta U^\dagger$:

$$W = -\beta^{-1}{\rm tr}[(\rho'_\beta - \rho_\beta)\log\rho_\beta] = \beta^{-1}S(\rho'_\beta|\rho_\beta) \ .$$

Suppose W is *completely* dissipated, i.e.: $\Delta S^{\rm th} = W/k_B T = \beta W$, hence:

$$\Delta S^{\rm th} = S(\rho'_\beta|\rho_\beta) \ > 0 \ .$$

We'll find $\mathcal{M}$ such that $\Delta S = \Delta S^{\rm th}$ for $V \to \infty$.

A graceful irreverzible map $\mathcal{M}$

$$\overbrace{\lim_{V\to\infty}\left[S(\mathcal{M}\rho'_\beta)-S(\rho_\beta)\right]}^{\Delta S}=\overbrace{\lim_{V\to\infty}S(\rho'_\beta|\rho_\beta)}^{\Delta S^{\mathrm{th}}}\ .$$

$\mathcal{M}$ is 'graceful' if it preserves the free dynamics of the reservoir:

$$\mathcal{M}\left[\mathrm{e}^{-itH}\rho\mathrm{e}^{itH}\right]\equiv\mathcal{M}\rho\quad\text{for all }\rho\ .$$

Hint from Maxwell gas (D. 2002), spin chain (D.,Feldmann,Kosloff 2006): $\mathcal{M}$ is complete permutation of molecules/spins.
This time we consider a correlated many-body system in box V with periodic boundary conditions. Let $U(x)$ *translate the frame* by the spatial vector x. (Don't confuse $U(x)$ with the local perturbation U.)
If the Hamiltonian is translation invariant, so is the equilibrium state:

$$U(x)HU(-x)\equiv H\quad\Longrightarrow\quad U(x)\rho_\beta U(-x)\equiv\rho_\beta\ .$$

The non-equilibrium state $\rho'_\beta=U\rho_\beta U^\dagger$ is not. For it, consider the following irreversible map:

$$\mathcal{M}\rho'_\beta=\frac{1}{V}\int_{x\epsilon V}U(x)\rho'_\beta U(-x)\mathrm{d}x\ .$$

This map is 'graceful' and *makes S increase by ΔS^{th}*.

Proof, 1st part

$$\lim_{V\to\infty}\left[S(\mathcal{M}\rho'_\beta) - S(\rho_\beta) - S(\rho'_\beta|\rho_\beta)\right] = 0 \ .$$

Extension of the rigorous method (of Csiszár,Hia,Petz 2007). Inspect the identity (from translation inv.):

$$S(\mathcal{M}\rho'_\beta|\rho_\beta) = -S(\mathcal{M}\rho'_\beta) + S(\rho'_\beta) + S(\rho'_\beta|\rho_\beta) \ .$$

Hence the eq. to be proven becomes:

$$\lim_{V\to\infty} S(\mathcal{M}\rho'_\beta|\rho_\beta) = 0 \ .$$

The Hiai-Petz (1991) lemma:

$$S(\sigma|\rho) \leq S_{BS}(\sigma|\rho) \ ,$$

where $S_{BS}(\sigma|\rho) = \mathrm{tr}[\sigma\log(\sigma^{1/2}\rho^{-1}\sigma^{1/2})]$ is the Belavkin-Staszewski relative entropy which one re-writes in terms of the function $\eta(s) = -s\log s$: $S_{BS}(\sigma|\rho) = -\mathrm{tr}[\rho\eta(\rho^{-1/2}\sigma\rho^{-1/2})] \geq 0$. Let us chain the Klein and the Hiai-Petz inequalities for $\sigma = \mathcal{M}\rho'_\beta$ and $\rho = \rho_\beta$:

$$0 \leq S(\mathcal{M}\rho'_\beta|\rho_\beta) \leq S_{BS}(\mathcal{M}\rho'_\beta|\rho_\beta) = -\mathrm{tr}[\rho\eta(\mathcal{M}E_\beta)] \ ,$$

where $E_\beta = \rho_\beta^{-1/2}\rho'_\beta\rho_\beta^{-1/2}$ and $\mathcal{M}E_\beta = \frac{1}{V}\int U(x)E_\beta U(-x)\mathrm{d}x$. If we prove $\mathcal{M}E_\beta = \mathrm{I}$ for $V\to\infty$, it means $\eta(\mathcal{M}E_\beta) = 0$. Then the above inequalities yield $S(\mathcal{M}\rho'_\beta|\rho_\beta) = 0$ for $V\to\infty$, which will complete the proof.

Proof, 2nd part

For $\mathcal{M}E_\beta = \mathrm{I}$, we use heuristic arguments. We consider second quantized formalism where all quantized fields satisfy $A(x,t) = \exp(itH)A(x)\exp(-itH)$. Assume pair-potential that vanishes at $> \ell$. It is plausible to assume that perturbations have a maximum speed v of propagation. Hence, at any given time t after the unitary perturbation $\rho'_\beta = U\rho_\beta U^\dagger$ e.g. around the origin, there exists a finite volume of radius r such that

$$[U, A(x,t)] = 0 \quad \text{for all } |x| > r$$

and for all local quantum fields $A(x,t)$. Let us write E_β in the form $E_\beta = \rho_\beta^{-1/2} U \rho_\beta U^\dagger \rho_\beta^{-1/2} = u_\beta u_\beta^\dagger$ with

$$u_\beta = \rho_\beta^{-1/2} U \rho_\beta^{1/2} = \mathrm{e}^{\beta H/2} U \mathrm{e}^{-\beta H/2} \ .$$

u_β is the (non-unitary) equivalent of U, transformed by the operator $\mathrm{e}^{\beta H/2}$. By analytic continuation $\beta \Rightarrow i\beta$ and because of finite speed of perturbations, the operator u_β and thus E_β, too, will commute with all remote fields: $[u_\beta, A(x,t)] = [E_\beta, A(x,t)] = 0$ provided $|x| \gg r + v\beta$. Take the infinite volume limit $V \to \infty$! Since the sub-volume where $A(x,t)$ do *not* commute with E_β is finite and since E_β is a bounded operator, the averaged operator $\mathcal{M}E_\beta$ will commute *with all fields* $A(x,t)$ for *all* coordinates x! Hence $\mathcal{M}E_\beta = \lambda\mathrm{I}$ and the identity $\mathrm{tr}(\rho_\beta \mathcal{M}E_\beta) = \mathrm{tr}(\rho_\beta E_\beta) = 1$ yields $\lambda = 1$.

Realistic versions of $\mathcal{M}$

Graceful irreversible map $\mathcal{M}$ at less artificial conditions: many-body system in infinite V.

$$\mathcal{M}\rho'_\beta = \lim_{R\to\infty} \frac{1}{8\pi R^3} \int \mathrm{e}^{-|x|/R} U(x)\rho'_\beta U(-x)\mathrm{d}x \ .$$

It's plausible that $\mathcal{M}$ makes the reservoir *forget* the information about the *location* of perturbation, that amounts exactly to the thermodynamic entropy production.

A real quantum reservoir would gracefully forget the *location* of perturbation. It does not need to forget it immediately; it may do it at any later time. It does not need to forget it completely; it may do it on a certain finite scale R of *spatial frame coarse-graining*. In concrete cases, the information loss can be well saturated at some finite scale $R \gg r + v\beta$. Instead of the spatial frame, the temporal one can be made forgotten:

$$\mathcal{M}\rho'_\beta = \lim_{\tau\to\infty} \frac{1}{\tau} \int_{-\infty}^{0} \mathrm{e}^{t/\tau} U(-t)\rho'_\beta U(t)\mathrm{d}t \ ,$$

where $U(t) = \exp(-iHt)$. This state is definitely different from the result of spatial averaging. Conjecture: for $\tau, V \to \infty$ it gains the same entropy.

Frameness

is about physical definiteness of a coordinate system.
Example: linear coordinates represented by spin chain (discret), or many-body system (continuous).
If the state is translation invariant (with periodic boundary), e.g.:

$$\rho = \sigma \otimes \sigma \otimes \sigma \otimes \sigma \otimes \sigma \otimes \sigma \otimes \sigma \otimes \cdots \otimes \sigma \ ,$$

$$\rho = \rho_\beta \quad \text{(Gibbs with } U(x)HU(-x) = H) \ ,$$

then *frameness*=0. If the state is translation non-invariant, e.g.:

$$\rho' = \sigma \otimes \sigma' \otimes \sigma \otimes \sigma \otimes \cdots \otimes \sigma \ ,$$

$$\rho' = U\rho_\beta U^\dagger \qquad \text{(local pert. of } \rho_\beta) \ ,$$

then *frameness*>0.
What could be the measure of frameness?

Twirl

A ‘closest’ invariant state by *twirl* $\mathcal{W}$:

$$\rho' \Rightarrow \mathcal{W}\rho' =: \frac{1}{V}\int_{x\epsilon V} U(x)\rho' U(-x)\mathrm{d}x \ .$$

Let frameness of ρ' be measured by twirl's entropy gain (Vaccaro, Anselmi, Wiseman & Jacobs, 2008):

$$F(\rho') = S(\mathcal{W}\rho') - S(\rho') \ .$$

Theorem (Gour, Marvian, Spekkens 2009):

$$S(\mathcal{W}\rho') - S(\rho') =: S(\rho'|\mathcal{W}\rho') \ .$$

So, the informatic measure of frameness is the relative entropy of the twirled state w.r.t. the state itself:

$$F(\rho') = S(\rho'|\mathcal{W}\rho') \ .$$

That's similar and related to the concept of the ‘graceful’ irreversible map $\mathcal{M}$, obtained from the principle of equivalence between thermodynamic and informatic entropy productions (Diósi, Feldmann, Kosloff 2007). For the simplest $\mathcal{M}$, we have $\mathcal{M} = \mathcal{W}$.

Summary

$$\lim_{V\to\infty}[S(\mathcal{M}\rho') - S(\rho')] = \lim_{V\to\infty} S(\rho'|\rho) \ ,$$

where $U(x)\rho U(-x) \equiv \rho$, $\rho' = U\rho U^\dagger$, and

$$\mathcal{M}\rho' = \frac{1}{V}\int_{x\epsilon V} U(x)\rho' U(-x)\mathrm{d}x \ .$$

This is a novel mathematical theorem for the entropy gain of complete frame averaging. We (DFK 2006) came to such conjecture by postulating a calculable model of both thermodynamic and von Neumann entropy gain. Mathematicians proved it, found it relevant to a certain quantum channel capacity problem (Csiszár, Hiai & Petz 2007). Others (Vaccaro et al, Gour et al), independently, found a related theorem to quantify the quality of reference frames (frameness):

$$S(\mathcal{M}\rho') - S(\rho') = S(\rho'|\mathcal{M}\rho') \quad \text{(for all } \rho') \ .$$

Nature would gracefully produce irreversibility just by twirling our reference frames (or, equivalently, by twirling matter). Then Nature is producing the observed thermodynamic irreversibility - at least in our calculable models. Whether this is the real and ultimate way for Nature to 'forget' microscopic data remains an open question.

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