von Neumann's "other" entropy: properties, interpretation, and applications

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Abstract

In addition to the quantity now eponymously known as von Neumann entropy, in his 1932 book von Neumann also discusses another entropic quantity, which he calls "macroscopic", and argues that it is the latter, and not the former, that is the relevant quantity to use in the analysis of thermodynamic systems. For a long time, however, von Neumann's "other" entropy was largely forgotten, appearing only sporadically in the literature, overshadowed by its more famous sibling. In this talk I will discuss a recent generalization of von Neumann's macroscopic entropy, called "observational entropy", focusing on its mathematical properties (leading to a strong version of the Petz recovery theorem), its statistical interpretation (as statistical deficiency on the one hand, and as "irretrodictability" on the other), and its application in explaining the emergence of the Second Law and an "H-like Theorem" for closed systems evolving unitarily.

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a growing list:
The Observational Entropy Appreciation Club
(www.observationalentropy.com)

von Neumann entropy

For $\varrho = \sum_{x=1}^{d} \lambda_x |\varphi_x\rangle\langle\varphi_x|$ d-dimensional density matrix ($\lambda_x \geq 0$, $\sum_x \lambda_x = 1$),

$$\boxed{S(\varrho) := -\operatorname{Tr}[\varrho \log \varrho] = -\sum_{x=1}^{d} \lambda_x \log \lambda_x}$$

with the convention $0 \log 0 := 0$.

Unfortunately though:

> *"The expressions for entropy given by the author [previously] are not applicable here in the way they were intended, as they were computed from the perspective of an observer who can carry out all measurements that are possible in principle—i.e., regardless of whether they are macroscopic [or not]."*

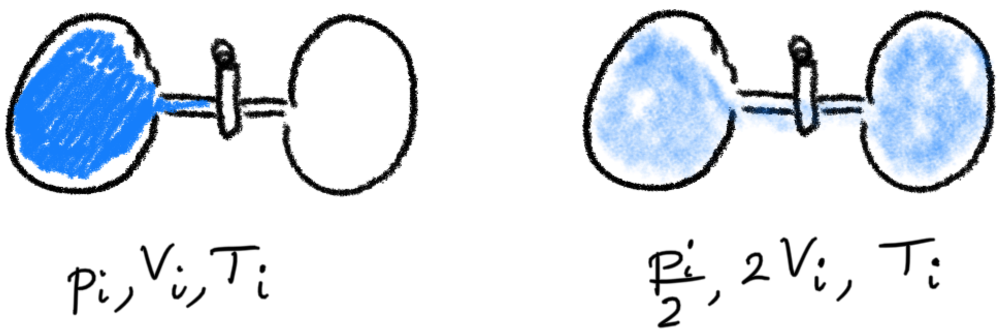
von Neumann, 1929; transl. available in `arXiv:1003.2133`

And again:

> *"Although our entropy expression, as we saw, is completely analogous to the classical entropy, it is still surprising that it is invariant in the normal [Hamiltonian] evolution in time of the system, and only increases with measurements—in the classical theory (where the measurements in general played no role) it increased as a rule even with the ordinary mechanical evolution in time of the system. It is therefore necessary to clear up this apparently paradoxical situation."*

von Neumann, book (Math. Found. QM), 1932 (transl. 1955)

the paradox: free expansion of an ideal gas



$$\boxed{\Delta S(\text{universe}) = nR\log 2 > 0}$$

$\Longrightarrow$ there is net entropy increase in an isolated system's evolution, but von Neumann entropy remains constant

von Neumann's insight (inspired by Szilard's)

"For a classical observer, who knows all coordinates and momenta, the entropy is constant. [...] The time variations of the entropy are then based on the fact that the observer does not know everything—that he cannot find out (measure) everything which is measurable in principle."

von Neumann, 1932 (transl. 1955)

von Neumann recognizes that thermodynamic entropy should be a quantity *relative* to the observer's knowledge

von Neumann's proposal: macroscopic entropy

For

- ϱ density matrix,
- $\mathbf{\Pi} = \{\Pi_i\}_i$ orthogonal resolution of identity (PVM),
- $p_i = \mathrm{Tr}[\varrho\, \Pi_i]$,
- $\Omega_i := \mathrm{Tr}[\Pi_i]$,

$$\boxed{S_{\mathbf{\Pi}}(\varrho) := -\sum_i p_i \log \frac{p_i}{\Omega_i}}$$

modern version: observational entropy

For

- ϱ density matrix,
- $\mathbf{P} = \{P_i\}_i$ POVM (i.e., $P_i \geq 0$, $\sum_i P_i = \mathbb{1}$),
- $p_i = \mathrm{Tr}[\varrho\, P_i]$,
- $V_i := \mathrm{Tr}[P_i]$,

$$\boxed{S_{\mathbf{P}}(\varrho) := -\sum_i p_i \log \frac{p_i}{V_i}}$$

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"observational" = "of the observer"

- von Neumann defines a **macro-observer** as a collection of simultaneously measurable quantities $\{\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n, \ldots\}$, where $\mathbf{X}_n = \{X_{j_n}\}_{j_n}$ are POVMs
- $\implies$ there exists one most-refined "parent" POVM $\mathbf{P} = \{P_{\boldsymbol{j}}\}_{\boldsymbol{j}}$ that outputs all values at once

$$X_{j_n} = \sum_{j_i \neq j_n} P_{j_1, j_2, \ldots, j_n, \ldots}\ , \quad \forall j, n$$

- hence, a macro-observer for von Neumann is "just" a POVM (i.e., the most-refined parent POVM $\mathbf{P}$) from which all macroscopic quantities can be simultaneously inferred

Properties of OE

Umegaki's relative entropy

Definition

For density matrices ϱ, γ,

$$D(\varrho\|\gamma) := \begin{cases} \mathrm{Tr}[\varrho(\log\varrho - \log\gamma)] \ , & \text{if } \operatorname{supp}\varrho \subseteq \operatorname{supp}\gamma \ , \\ +\infty \ , & \text{otherwise} \end{cases}$$

Useful properties:

- $D(A\|B) \geq 0$
- $S(\varrho) = \log d - D(\varrho\|u)$ where $u := d^{-1}\mathbb{1}$
- **monotonicity**: $D(\varrho\|\gamma) \geq D(\mathcal{N}(\varrho)\|\mathcal{N}(\gamma))$ for all channels (i.e., CPTP linear maps) $\mathcal{N}$ and all states ϱ, γ

the fundamental bound of OE

Theorem (arXiv:2209.03803)

For d-dimensional quantum system, density matrix ϱ, and POVM $\mathbf{P} = \{P_i\}_i$:

$$T\ln(d-1) + h(T) \geq S_{\mathbf{P}}(\varrho) - S(\varrho) \geq D(\varrho\|\tilde{\varrho}_{\mathbf{P}}) ,$$

where

- $\tilde{\varrho}_{\mathbf{P}} := (\mathcal{R}^u_{\mathcal{P}} \circ \mathcal{P})(\varrho) = \sum_i \mathrm{Tr}[\varrho\ P_i]\,\frac{P_i}{V_i} \rightsquigarrow$ *reconstructed state*
- $\mathcal{R}^u_{\mathcal{P}}(\cdot) := \frac{1}{d}\mathcal{P}^\dagger[\mathcal{P}(u)^{-1/2}(\cdot)\mathcal{P}(u)^{-1/2}] \rightsquigarrow$ *Petz transpose map*
- $T := \frac{1}{2}\|\varrho - \tilde{\varrho}_{\mathbf{P}}\|_1$
- $h(x) := -x\ln x - (1-x)\ln(1-x)$

Remark. If $S_{\mathbf{P}}(\varrho) = S(\varrho)$, the state ϱ is said to be macroscopic for observer **P**.

Remark. In general, it could be $[\varrho, \tilde{\varrho}_{\mathbf{P}}] \neq 0$.

What is $\tilde{\varrho}_{\mathbf{P}}$?

The state $\tilde{\varrho}_{\mathbf{P}} = \sum_i \mathrm{Tr}[\varrho\ P_i]\,\frac{P_i}{V_i}$:

- only depends on the observer's knowledge
- it is the coarse-grained state that appears in Gibbsian "proofs" of the second law
- it is the retrodiction or quantum Bayes' inverse done by the observer about the "true" (but unknown) microscopic state of the system

parenthesis: Watanabe's contention

"The phenomenological oneway-ness of temporal developments in physics is due to irretrodictability, and not due to irreversibility."

Satosi Watanabe (1965)

The difference $S_{\mathbf{P}}(\varrho) - S(\varrho)$ is precisely a measure of such an irretrodictability.

A law of OE increase in isolated systems

an "H theorem" for OE

Theorem (arXiv:2404.11985)

In a d-dimensional system, choose a state ϱ and a POVM $\mathbf{P} = \{P_i\}_i$ with a finite number of outcomes. Choose also a (small) value $\delta > 0$. For a unitary operator U sampled at random according to the Haar distribution, it holds:

$$\mathbb{P}_H \left\{ \frac{S_{\mathbf{P}}(U \varrho U^\dagger)}{\log d} \leq (1-\delta) \right\} \leq \frac{4}{\kappa(\mathbf{P})} e^{-C\delta\kappa(\mathbf{P})^2 d \log d} ,$$

where $\kappa(\mathbf{P}) = \min_i \mathrm{Tr}[P_i\, u]$ and $C \approx 0.0018$.

Remark. A similar statement holds for unitaries sampled from an approximate 2-design.

$\Longrightarrow$ in the eyes of the observer, the state of a randomly evolving system **quickly** becomes **indistinguishable** from the maximally uniform one, regardless of the system's initial state.

Conclusions

take-home messages

When the use of von Neumann entropy in thermodynamics is problematic, try consider observational entropy (OE) instead, because:

1. OE has a fully operational/inferential definition
2. OE fits nicely within recent developments in quantum mathematical statistics (e.g., approximate Petz recovery, strengthened monotonicity bounds, etc.)
3. OE simplifies a number of conceptual issues within the foundations of statistical mechanics

The End: Thank You!

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