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A unified entropy for statistical mechanics: observational entropy meets maximum entropy principles

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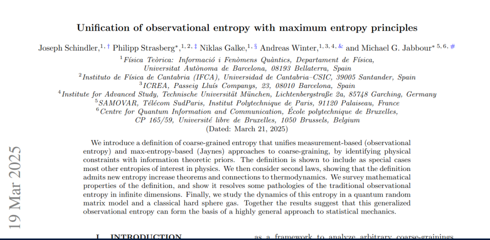

19 Mar 2025

Unification of observational entropy with maximum entropy principles

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(Dated: March 21, 2025)

We introduce a definition of coarse-grained entropy that unifies measurement-based (observational entropy) and max-entropy-based (Jaynes) approaches to coarse-graining, by identifying physical constraints with information theoretic priors. The definition is shown to include as special cases most other entropies of interest in physics. We then consider second laws, showing that the definition admits new entropy increase theorems and connections to thermodynamics. We survey mathematical properties of the definition, and show it resolves some pathologies of the traditional observational entropy in infinite dimensions. Finally, we study the dynamics of this entropy in a quantum random matrix model and a classical hard sphere gas. Together the results suggest that this generalized observational entropy can form the basis of a highly general approach to statistical mechanics.

I. INTRODUCTION

as a framework to analyze arbitrary coarse-grainings

(Broader-audience version in preparation.)

arxiv:2503.15612

ENTROPY

Its perpetual increase is at the center of almost all everyday phenomena.

It cools our coffee.

It kills our pets.

It's the enemy of demons everywhere.

But what the hell is it??

The main problem is that **no one can agree on what it means**.[1]

- Gibbs says it's $S = \int d \quad \log \quad$.
- Boltzmann says it's $S = k \log W$.
- Gibbs says it's $S = \int d \quad {}_{\mathrm{cg}} \log \quad {}_{\mathrm{cg}}$.
- Boltzmann says it's $S = \int dxdp\, P(x;p) \log P(x;p)$.
- von Neumann says it's $S = \mathrm{Tr} \quad \log \quad$.
- von Neumann says it's $S = \sum_i p_i \log(p_i/V_i)$.

OQS Classical Textbooks HEP

[1] We're talking physics, not information theory. Informational things like Rényi entropies, conditional entropies, or f-divergences, are well understood and not part of this confusion.

The main problem is that **no one can agree on what it means**.[1]

- Open Quantum Systems says it's $S = S(\ (t))$ (von Neumann entropy of the microscopic state).
- Equilibrium Statistical Mechanics says it's $S = S(\ (t))$ (von Neumann entropy of the micro-/canonical/etc ensemble).
- Classical systems equilibration says it's $S = k \log W$ (number of microstates in a macrostate).
- Isolated quantum equilibration says it's an observable entropy with the system viewed through a measurement M.

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The main problem is that **no one can agree on what it means**.[1]

- Isolated quantum systems say it's the diagonal entropy.
- Isolated quantum systems say it's the observable Shannon entropy.
- Isolated quantum systems say it's the observational entropy.
- Some prefer the entanglement entropy.

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The main problem is that **no one can agree on what it means**.[1]

- Quantum thermodynamics says it's
  $S = D(\ (t)k\ _S(t)\ \ \ _B(t))$.

- Stochastic thermodynamics says it's
  $S = \ \ \ hE_x i + \ hS_x \ \ \log p_x i$.

- Thermodynamics says it's
  $dS = dQ{=}T$.

- And the list goes on...

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The main problem is that **no one can agree on what it means**.[1]

- *Nearly all the entropies discussed have at some point been treated as "the" entropy of statistical thermodynamics, leading to a century of debate about which one is "correct" or "fundamental".*
- *Each one looks correct in some regime.*
- Which one could it be?

OQS Classical Textbooks HEP

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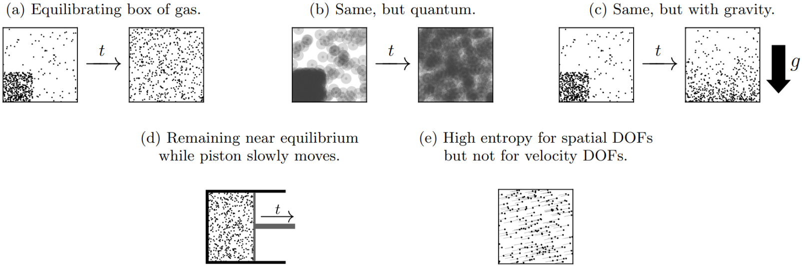
Can any of these be the **general** definition of entropy?



Some of the most common candidates:

7 von Neumann entropy of microstate $S(\ (t))$ A,B
7 von Neumann entropy of equilibrium ensemble $S(\ (t))$ A,B
7 Boltzmann entropy $\log W$ B
7 Shannon observable entropy $H_M(\ )$ A,C
7 Observational entropy $S_M(\ )$ C

And the rest fail too, or are not even defined in all these cases.

A **general** entropy should:

- Make the 2nd law of Thermodynamics = Law of Entropy Increase, for *all* physical manifestations of 2nd law.
- Allow one to to **prove** entropy increase under suitable assumptions.
- **Connect** entropy increase to physical consequences, like "heat flows from hot to cold bodies" or "a gas fills its container".

- Gas in a box expands to uniformly ll its container.
- Heat ows from hot to cold bodies, in both classical and quantum systems.
- Glass does not unshatter, but oil separates when mixed with water.
- An isolated quantum pure state thermalizes with respect to observables.
- An open quantum system thermalizes at the level of its density matrix.
- Thermodynamic cycles, both classical and quantum, have limited e ciency.
- A piston does piston things with gas and work.
- A chemical reaction proceeds spontaneously.

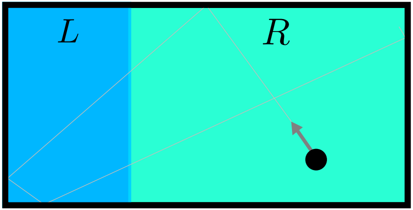
Not all systems equilibrate. But one should be able to prove it \where appropriate".
The proofs should help clarify precisely when equilibration does/doesn't occur.

Increase of a quantity called entropy is not enough to be a 2nd Law.
It has to connect to the physics.

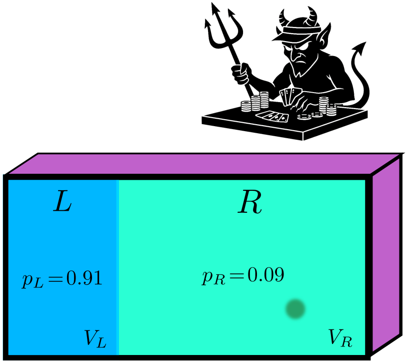
In this talk I'll give a general entropy definition that has **all of the entropies discussed earlier** as special cases or limits, explain the motivations behind it, and say what it could suggest about 2nd laws and equilibration.

Balls and Boxes

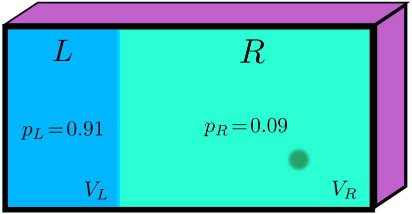
A ball is in a box.
The box has a left and right side.



Now I hide the ball.
But I give you the probability that I put it in the left or right.



If you tell me ball is definitely on the right, I have uncertainty $\log V_R$ about where precisely the ball is. Telling me the smaller box gives me more info.



How much uncertainty do I have about...

Which box is the ball in?

$$\sum_i p_i \log p_i$$

Shannon observable entropy

Where is the ball?

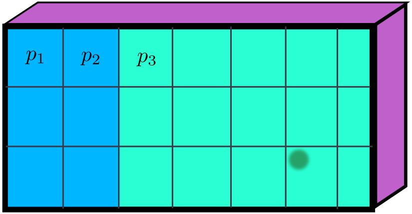
$$\sum_i p_i \log p_i + \sum_i p_i \log V_i$$

Observational entropy

Information about the outcome vs. information about the state.

OE = uncertainty about which box + uncertainty given the particular box

Refining the measurement ! better information about where the ball is.

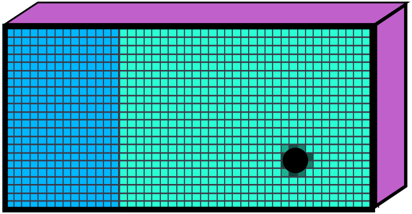


CPTP monotonicity of relative entropy ! coarser/finer monotonicity of OE

$$S\ \ _M(\ )\quad S_M(\ )$$

(aka data processing inequality)

If the location of the ball has *inherent* uncertainty (finite size of ball), the finest possible measurements reveal this minimum amount.



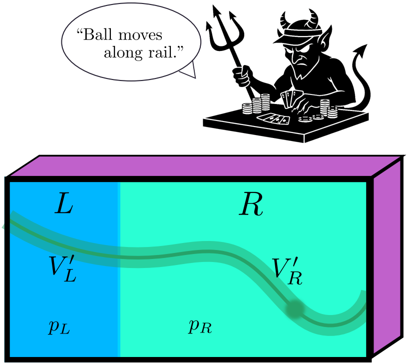
Observer's uncertainty (OE)   inherent uncertainty in state ($S($ $)$ =   log)

$$S_M(\rho) \geq S(\rho)$$

Optimal measurements (eigenbasis) reveal von Neumann entropy.

Now I give you some additional info by telling you a constraint.

(Energy conservation, charge conservation, restriction to a subspace...)



Learning “right box” fixes the location more than before *!*
recalculate volumes in light of the constraint.

Given both constraint info + measurement outcome probabilities,
new uncertainty: $\sum_i p_i \log p_i + \sum_i p_i \log V_i'$

Combining constraints + measurement makes this entropy unification possible.

Formal De nition

The state of the system is .

I have two pieces of \coarse information" about :

- I know it obeys some particular constraint $\mathrm{Tr}(X) = 0$,
- I know the outcome statistics $p_i = \mathrm{Tr}(M_i)$ of a POVM $M = (M_i)_i$.

How much uncertainty do I have?

First, I estimate using the maximum entropy principle, getting \prior" .

- = MaxEnt state given the constraint (maximum vN entropy)

This leaves me with uncertainty $S( ) = \mathrm{Tr} \log$ about the state.

Next I calculate my prior estimate $q_i = \mathrm{Tr}(M_i)$ of the M outcomes.

In classical information theory, the informational value (in bits saved) of learning p_i, when previously I had the prior q_i is $D(p \| q)$.

So gaining knowledge of M info decreases my uncertainty to

$$S_M ( ) = S( ) \; D_M (\|):$$

For example:

The state of the system is $= |3\rangle\langle 3|$.
Hamiltonian is $H = \sum_k k|k\rangle\langle k|$.

You tell me the constraint $\langle H\rangle = E$.
I make my best (maxent) guess at , which is $= \frac{e^{\ H}}{Z}$ with some .
Current uncertainty $S(\ ) = \log Z + \ E$.

You give me data of the measurement $M = (|k\rangle\langle k|)_k$ (energy eigenbasis).
My guess would have been $q_k = \mathrm{Tr}(\ \ _k) = e^{\ E_3}/Z$:
The actual data is $p_k = \mathrm{Tr}(\ \ _k) = \ _{k;3}$.
I gained $D_M(\ \|\ ) = D(p\|q) = \ \log q_3$ bits of information.

My total uncertainty is

$$S_M(\ ) = \log Z + \ E \quad D_M(\ \| e^{\ H}/Z)$$

De nition. The entropy of state , coarse-grained by measurement M, with prior , is

$$S_M(\ ) = S(\ )\ \ D_M(\ k\ ):$$

This is missing information given both measured info and constraint info.

Prior = MaxEnt state for constraints on the system.
Measured RE: $D_M(\ k\ )$ $D(p k q)$ where $p_x = \mathrm{Tr}(M_x\ )$ and $q_x = \mathrm{Tr}(M_x\ )$.

\Entropy = Missing Information." Compare

$$H(p) = \log N \quad D(p k 1{=}N)$$
$$S(\ ) = \log d \quad D(\ k 1{=}d)$$
$$S_M(\ ) = \log d \quad D_M(\ k 1{=}d):$$

These implicitly assume prior ignorance, with uniform prior 1=d.

Explicitly,

$$D_M(\ k\ ) \quad \overset{X}{\underset{x}{}} \ \mathrm{Tr}(M_x\ ) \log \frac{\mathrm{Tr}(M_x\ )}{\mathrm{Tr}(M_x\ )}$$

Equivalent de nition. The above entropy is equivalent to

$$S_M(\ ) = \sum_x p_x \log \frac{p_x}{V_x};$$

which is also the Shannon plus mean Boltzmann entropy

$$S_M(\ ) = H(p) + \textstyle\sum_x p_x \log V_x;$$

combining \which macrostate" uncertainty and \which microstate given the macrostate" uncertainty.

Macrostate probabilities (actual and prior): $p_x = \mathrm{Tr}(M\ \ _x\ )$ and $q_x = \mathrm{Tr}(M\ \ _x\ )$.
E ective dimension of set of constrained states: $d_e = e^{S(\ )}$.
Macrostate volumes: $V_x = q_x\, d_e$.

Volumes = prior macrostate probabilities * e ective dimension of constrained state space

Di erent M capture di erent ways a state can be low entropy!

Equilibrium: High entropy for \all" coarse M.
Ability to do M that reveals low entropy ! extract resources from the system.

(Depicted: Prior = e^{H} =Z, Measurement M = spatial, velocity, speeds, or thermodynamic.)

(poster)

Lot's more to say! But let's skip to equilibration.

2nd Laws, Equilibration, Thermalization

The map of second laws.

- Say (t) equilibrated if looks like $\bar{}$ to all coarse M.
- Say (t) thermalized if looks like = e^{H} =Z to all coarse M.
- Say (t) equilibrated to if looks like to all coarse M.

Thermalization is common. Example:

(animation)

Challenge:

Tell me a coarse M now, that after time t will distinguish from $= e^{H} = Z$.

Not unique: could equally well say microcanonical $= {}_E = W_E$.

A fun connection.

You can't distinguish between the particles.
You can only do M that measures distributions of 1p properties
(think Max-Boltz speed distribution).

The M measuring $P(x;p)$ from Boltzmann's H-theorem is finer than all the other such M. Thus for any M you can do

$$\min_{M \in \{\text{avalailable } M\}} S_M(\ ) = S_{M_{P(x;p)}}(\ )$$

where

$$S_{M_{P(x;p)}}(\ ) = C \quad n \int dxdp\, P(x;p) \log P(x;p).$$

(animation)

Boltzmann's H-theorem proves an observer would at least need to distinguish between particles to possibly reveal low entropy.

*Ask me about Gibbs H-theorem and why QM thermalization is more robust.

A quantum example of thermalization and its classical counterpart.

Both just look like \weakly coupled heat exchange".

Is chaos necessary? (What we see so far...)

Non-integrable systems will generically thermalize for all ICs and all coarse M.

Free systems will appear to thermalize for some ICs and some M, but not others.

Free systems likely do equilibrate to $\bar{}$ generically, but not to some useful looser .

animations

Theory of equilibration

Isolated system equilibration

Deviation from maximal entropy is

$$(t) = D_M ((t) k):$$

Second Law on Average

Equilibration to on average if

$$= \overline{D_M (k)} :$$

Key Theorem.

$$\overline{D_M (k)} = \overline{D_M (k \bar{})} + D_M (\bar{} k):$$

Equilibration term + Thermalization term.

Equilibration if is tight enough and M is coarse enough.

First term: Dynamical bounds.
Second term: ETH-like things.

Equilibration term $\overline{D_M(\ k\ \bar{)}}$

3 Large Systems Bound

Many more occupied energy eigenstates than number of measurement outcomes ($d_2(\bar{)}$ m).

$$\overline{D_M(\ k\ \bar{)}}\quad \log m + g(\ );$$

where $=\ \frac{p}{4}\frac{m}{d_2(\bar{)}}$.

3 Small Systems Bound

Just a few occupied energy eigenstates ($S(\bar{)}$ $S(\ )$).

$$\overline{D_M(\ k\ \bar{)}}\ \ S(\ \ \bar{)}:$$

$d_2(\bar{)} = 1{=}\mathrm{Tr}(\ \ \bar{\ }^2)$
$g(\ ) = \ \log\ + (1+\ )\log(1+\ )$

... Medium Systems ????

Numerics suggest more bounds exist.

Thermalization term $D_M(\bar{} k\ )$

\Measured ergodic hypothesis"

3 Simple bound.

Time-averaged probabilities similar to prior probabilities.

$$D_M(\bar{} k\ ) \quad \log \sup_x \frac{\overline{p_x(t)}}{q_x}$$

3 ETH Bound

Nearby energy eigenstates look the same to M.

Suppose $D_M(\ _E\ k\ _{E'}) \quad _{eth}$ for all $E; E'$ in the relevant energy window. Then

$$D_M(\bar{} k\ ) \quad _{eth} :$$

To break integrable systems look at therm term.

Fewer M will obey ETH?

$H = H_A + H_B + H_{int}$
weak coupling

$= e^{\ H} = Z$
energy conservation

$M = M_{E_A} \quad M_{E_B}$
coarse local energy measurements

From entropy increase to physical consequences

Suppose we successfully proved $\overline{D_M(k)}$ using methods of previous section, for coarse local energy measurement $M = M_A \quad M_B$ with thermal prior $= e^{\ H} =Z$.

- Note: Empirically true in the numerical example.

Consider the systems on the left.
Assume quantum uncertainty is less than energy bin widths, so that $M_{E_A} \quad M_{E_B}$ gives a single de nite outcome.
Take weak coupling limit.

Then you can prove the observed energies will obey

$$dS_M = \frac{dE_A}{T_A} + \frac{dE_B}{T_B} > 0;$$

and that equilibrium is at

$$T_A = T_B\,;$$

with $T^{1} = \frac{@}{@E} \log W_E$ textbook Boltzmann temps.

Heat ows from hot to cold bodies!

You need the special new V_E for the equilibration proof, but standard W_E come out for weak coupling.

Concluding Remarks

If only we had more time. I haven't yet mentioned:

- The hierarchy of constraints and constraint/state bijection.
- Connections to entanglement theory.
- Connections to quantum measurement theory.
- Connections to Bayesian state estimation problems.
- Entropic uncertainty principles.
- ...

There are loads of open questions! Including:

- Strengthening and applying equilibration/thermalization bounds.
- Free vs chaotic.
- How can you extract resources given ability to reveal low entropy?
- Fluctuation theorems.
- OK I'm running out of time...

Please help!! ;)

Von Neumann writes

It remains to define the entropies of ψ and $\mathbf{U}_\psi$ (of the state and of the corresponding (virtual) micro-canonical ensemble). The expressions for entropy given by the author in [20] 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 (for example, there every pure state has entropy 0, only mixtures have entropies greater than 0!). If we take into account that the observer can measure only macroscopically then we find different entropy values (in fact, greater ones, as the observer is now less skilful and possibly can therefore extract less mechanical work from the system); nevertheless, the theory can be set up also in this case. How to do this has been discussed by E. Wigner.[31] the formulas for the entropies $S(\psi), S(\mathbf{U}_\psi)$ of ψ and $\mathbf{U}_\psi$ read:[32]

$$S(\psi) = -\sum_{a=1}^{\infty}\sum_{\nu=1}^{N_a}(\mathbf{E}_{\nu,a}\psi,\psi)\ln\frac{(\mathbf{E}_{\nu,a}\psi,\psi)}{s_{\nu,a}}, \tag{34}$$

$$S(\mathbf{U}_\psi) = -\sum_{a=1}^{\infty}(\mathbf{\Delta}_a\psi,\psi)\ln\frac{(\mathbf{\Delta}_a\psi,\psi)}{S_a}. \tag{35}$$

By the way, these entropy formulas are identical to the usual ones based on Boltzmann's definition of entropy (and Stirling's formula), as one sees by noting that the $(\mathbf{E}_{\nu,a}\psi,\psi)$ (the $(\mathbf{\Delta}_a\psi,\psi)$) are the relative occupation numbers of the phase cells (of the energy surfaces) and the $s_{\nu,a}$ (the S_a) are the numbers of quantum orbits therein, i.e., their so-called a-priori weights.

(*Proof of the Ergodic Theorem and the H-Theorem...*, 1929)

4. THE MACROSCOPIC MEASUREMENT

Although our entropy expression, as we saw, is completely analogous to the classical entropy, it is still

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surprising that it is invariant in the normal evolution in time of the system (process 2.), and only increases with measurements (process 1.) -- 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.

The normal classical thermodynamical considera-
tion runs as follows: One could take a container of

(*Mathematical Foundations* Book, Sec. V.4, 1955)

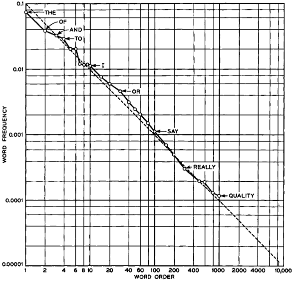
Statistical Thermo ! Entropy seen by observers
(in particular he uses what is now called observational entropy)

Final thought: A reminder about Shannon entropy

Prediction and Entropy of Printed English

By C. E. SHANNON

(*Manuscript Received Sept. 15, 1950*)



- *The entropy of (information in) a text depends on the decoding mechanism...* ...molecules, symbols, n-grams, words, meanings?
- Physical entropy also depends on the decoding mechanism.

	F_0	F_1	F_2	F_3	F_{word}
26 letter.................	4.70	4.14	3.56	3.3	2.62
27 letter.................	4.76	4.03	3.32	3.1	2.14

Thanks!

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