A unified entropy for statistical mechanics

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Main Definition

"What is entropy?"... What entropy definition can give a unified picture of the 2nd Law across non-/equilibrium, open/isolated, pure/mixed, classical/quantum systems?

The idea of this paper [1] is to combine von Neumann's "macroscopic entropy" [2] (*i.e.* "observational entropy" [3]) and Jaynes' "maximum entropy principle" [4] into a single coarse-grained entropy definition uniting nearly all entropies in physics.

Informational Form

Definition. The entropy of state ρ, coarse-grained by measurement M, with prior τ, is

$$S_M^\tau(\rho) = S(\tau) - D_M(\rho\|\tau).$$

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

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

The definition derives from the principle "entropy = missing information", or

$$S = I_{\text{tot}} - I,$$

which for Shannon $H(p)$, von Neumann $S(\rho)$, and the standard OE $S_M(\rho)$, is stated

$$H(p) = \log N - D(p\|1/N)$$
$$S(\rho) = \log d - D(\rho\|\mathbb{1}/d)$$
$$S_M(\rho) = \log d - D_M(\rho\|\mathbb{1}/d).$$

These implicitly assume prior ignorance, with $\mathbb{1}/d$ appearing as the informational prior. The new definition assumes prior knowledge of a linear constraint such as $\langle H\rangle = E$, with the maximum entropy state τ taken as the prior.

vN's macroscopic entropy (=traditional OE): $S_M(\rho) = \log d - D_M(\rho\|\mathbb{1}/d)$.

Stat Mech Form

Equivalent definitions. The above entropy is equivalent to

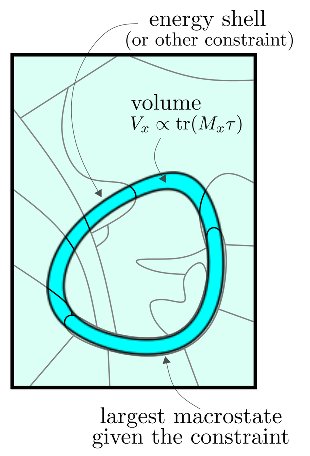
$$S_M^\tau(\rho) = -\sum_x p_x \log \frac{p_x}{V_x},$$

which is also the Shannon plus mean Boltzmann entropy

$$S_M^\tau(\rho) = H(p) + \textstyle\sum_x p_x \log V_x,$$

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

Macrostate probabilities (actual and prior): $p_x = \mathrm{Tr}(M_x\rho)$ and $q_x = \mathrm{Tr}(M_x\tau)$.
Effective dimension of set of constrained states: $d_{\text{eff}} = e^{S(\tau)}$.
Macrostate volumes: $V_x = q_x\, d_{\text{eff}}$.



Uniform *(Prior: $\tau = \mathbb{1}/d$. Constraint = trivial. Vols: $V_x = \mathrm{Tr}(M_x)$.):*

$$S_M^\tau(\rho) = \log d - D_M(\rho\|\mathbb{1}/d).$$

Canonical *(Prior: $\tau = e^{-\beta H}/Z$. Constraint $\langle H\rangle = E$. Vols: $\mathrm{Tr}(M_x e^{-\beta(H-E)})$.):*

$$S_M^\tau(\rho) = \beta E + \log Z - D_M(\rho\|e^{-\beta H}/Z).$$

Microcanonical *(Prior: $\tau = \Pi/W$. Constraint $\rho \in \Pi$. Vols: $V_x = \mathrm{Tr}(M_x\Pi)$.):*

$$S_M^\tau(\rho) = \log W - D_M(\rho\|\Pi/W).$$

...textbook EQ entropies become dynamical non-EQ maxima.

Entropy increase: system finds *most likely macrostates given the constraints*.

Observed versus Inherent Information

For states ρ obeying the constraint $S(\rho;\tau) \le S(\tau)$ (= arbitrary linear constraint),

$$S_M^\tau(\rho) \ge S(\rho).$$

No observer can extract more information than what is inherently available in the state.

Uniting the Entropy Zoo: Special Cases and Limits

Nearly all commonly used physical entropies derive from $S_M^\tau(\rho)$ as special cases and limits.

Fundamental Limits

- **von Neumann (or classical Gibbs) entropy** $S(\rho)$
  The lower bound $S_M^\tau(\rho) \ge S(\rho)$.
  Optimal M case: $\min_M S_M(\rho) = S(\rho)$.
  (Bound assumes constraint: false info is unbounded.)
- **Jaynes max entropy** $S(\tau)$
  The upper bound $S(\tau) \ge S_M^\tau(\rho)$.
  The equilibrium value.
  The case of trivial $M = (\mathbb{1})$.
- **Boltzmann entropy** $\log V_x$
  The case of a definite macrostate (only one nonzero p_x).
  In itself still a generalization due to generalized V_x.
  A contribution to the total (mean Boltzmann term).
- **Observable Shannon entropy** $H_M(\rho)$
  The case of equal prior probabilities ($V_x = const$),
  as for $M = (|x\rangle\langle x|)_x$ with $\tau = \mathbb{1}/d$.
  A contribution to the total (Shannon term).
- **Observational entropy (traditional def)** $S_M(\rho)$
  The case $\tau = \mathbb{1}/d$ (uniform prior, trivial constraint).

Entropy Production

- **Entropy production (general)**

  Large class of methods, often captured by

  $$\Delta S_M^\tau = S_{M_t}^{\tau_t}\big(\rho(t)\big) - S_{M_0}^{\tau_0}\big(\rho(0)\big)$$

  with time-dependent M, τ, ρ.
- **Entropy production (Quantum Thermo eg Potts 2019)**
  System $\otimes$ Bath
  $\tau(t) = \mathbb{1}_S \otimes \frac{e^{-\beta(t)H_B}}{Z}$ is bath energy constraint $\langle H_B\rangle = E_B(t)$.
  $M(t) = M_S(t) \otimes \mathbb{1}_B$ are optimal measurements on system.
  With $T_B = \beta^{-1}$ one finds

  $$\Delta S_M^\tau = \Delta S(\rho_S) + \int_0^t \frac{dE_B(t')}{T_B(t')}$$

  For decorrelated thermal $\rho(0)$ this equals the usual RE form, and is ≥ 0.
  Usual RE form is EP $= D(\rho(t)\|\rho_S(t) \otimes \tau_B(t))$.
- **Entropy production (Stochastic thermodynamics)**
  System $\otimes$ Environment.
  $\tau = \Pi_E/W_E$ global microcanonical energy shell.
  $M = \Pi_S \otimes \mathbb{1}$ projective measurement on system.
  Defining a bunch of fancy things shows

  $$\Delta S_M^\tau(\rho) = -\beta\Delta\langle E_x\rangle + \Delta\langle S_x - \log p_x\rangle$$

  which is stochastic EP as in (11) of Seifert 2017.

  S_x = intrinsic mesostate entropy
  E_x = mesostate energy
  β = environment temp

Local Detailed Balance

- **2nd law of stochastic thermodynamics**
  If $dp_x/dt = \sum_{x'} R_{xx'}p_{x'}$ with LDB $R_{xx'}/R_{x'x} = q_x/q_{x'}$, then

  $$\frac{d}{dt}S_M^\tau(\rho) = \sum_{x,x'} R_{xx'}p_{x'} \log \frac{R_{xx'}p_{x'}}{R_{x'x}p_x} \ge 0.$$

Clausius Relations

- **Clausius inequalities**
  See paper for how relations like

  $$\Delta S_M^\tau(\rho) = \int \frac{dE_A}{T_A} + \int \frac{dE_B}{T_B} \ge 0$$

  are derived in either canonical or microcanonical form, and conditions where ≥ 0 is guaranteed or highly probable.

More Particular Limits

- **Diagonal entropy**
  Boring version: The case $M = (|E\rangle\langle E|)_E$ with $\tau \propto \mathbb{1}$.
  Cool version: Equilibrium entropy $S(\overline{\rho})$ associated with the tightest possible stationary constraint $\tau = \overline{\rho}$.
  (Note: constant in isolated systems.)
- **Entanglement entropy**
  Minimum for local M on entangled subsystems,

  $$S_{\text{ent}}(\psi_{AB}) = \inf_{M_A, M_B} S_{M_A\otimes M_B}(\psi_{AB}).$$

  Compare global minimum $S(\rho) = \min_M S_M(\rho)$.
- **Wehrl entropy** (Wehrl 1979)
  The case of POVM $M = \left(\frac{|z\rangle\langle z|}{\pi}\right)_{z\in\mathbb{C}}$, where $|z\rangle$ are the overcomplete basis of coherent states, with $\tau \propto \mathbb{1}$, so

  $$S_M^\tau(\rho) = -\tfrac{1}{\pi}\int dz\, Q \log Q, \quad Q(z) = \langle z|\rho|z\rangle.$$
- **Free energies**
  Can arise in many ways, see paper.
- **Rényi, Tsallis, and related entropies**
  Replace D_M by generalized divergence. For Rényi,

  $$S_{M,\alpha}^\tau(\rho) = S(\tau) - D_M^\alpha(\rho\|\tau) = -\log \left\langle (p_x/V_x)^s \right\rangle_{p_x}^{1/s}$$

  where $\alpha = 1 + s$, measures moments of prob-to-vol ratio.
- **Dynamical canonical entropy**
  The case $\tau(t) \propto \tau_A(t) \otimes \tau_B(t)$ with $\tau_A(t) \propto e^{-\beta_A(t)H_A}$, and so on, for local energy constraint in subsystems.
- **HEP coarse-/fine-grained entropies**
  The cases $S(\tau)$ and $S(\rho)$, respectively.

Historical H-theorems

- **Boltzmann's H-theorems** (Boltzmann 1872)
  $\tau = e^{-\beta H}/Z$ canonical prior (average energy conservation).
  $M_{P(E)}$ measures distribution of 1-particle energies.
  $M_{P(\vec{x},\vec{p})}$ measures distribution over 1-particle phase space.

  $$S_{M_{P(E)}}^\tau(\rho) = C' - n\int P(E) \log \frac{P(E)}{E^{-\frac{d}{2}+1}}\, dE$$

  $$S_{M_{P(\vec{x},\vec{p})}}^\tau(\rho) = C - n\int P(\vec{x},\vec{p}) \log P(\vec{x},\vec{p})\, d\vec{x}d\vec{p}$$

  Therefore Boltzmann's H-theorems are equivalent to

  $$\frac{d}{dt}S_M^\tau(\rho) \ge 0.$$

  (Strict non-negativity is due to his simplifying assumptions.)
- **Gibbs H-theorem** (XII of Gibbs 1902)
  Uniform prior $\tau \propto \mathbb{1}$.
  M cuts the full n-particle phase space into finite cells.
  Equivalent to

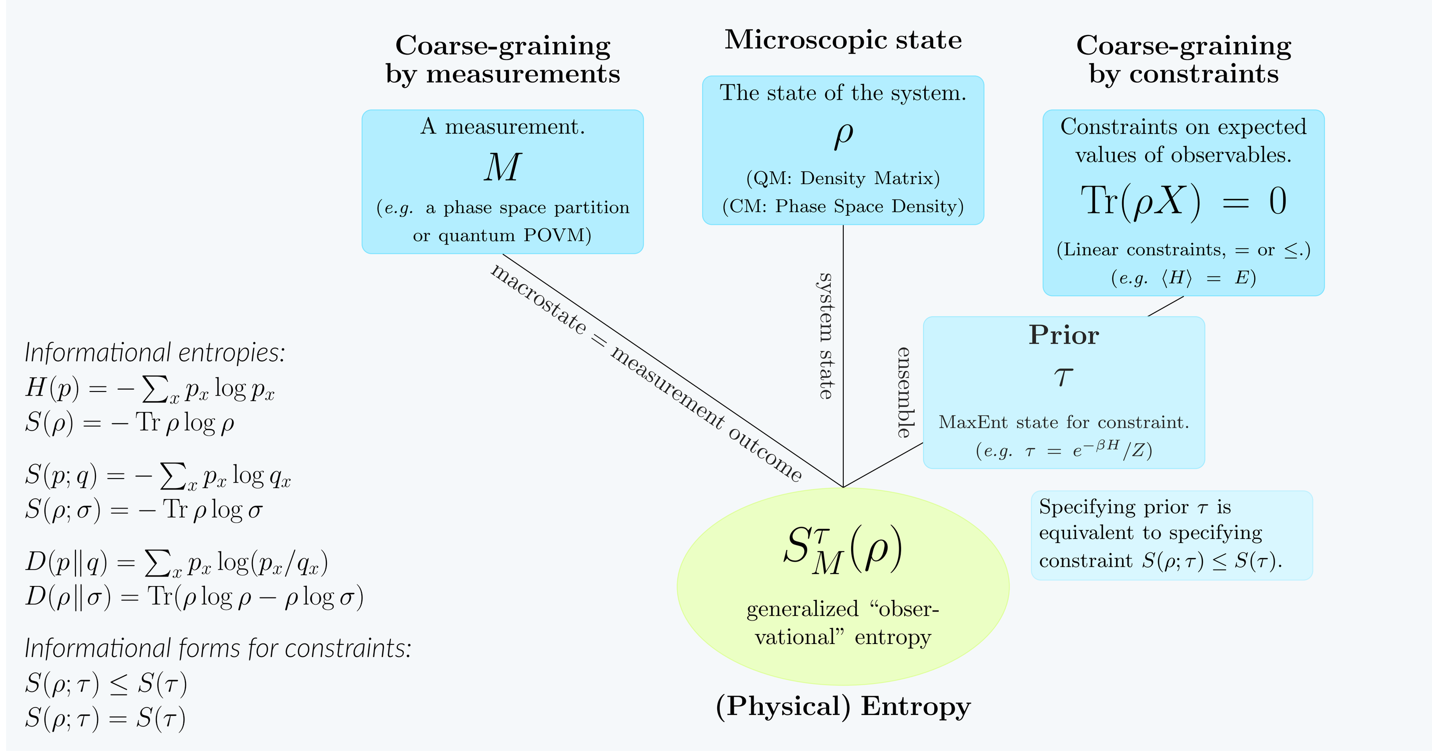
  $$S_M(\rho_0) \le S_M(\rho_{t\to\infty})$$

  in notation of (66-67) of Ehrenfest 1912.
- **von Neumann's quantum H-theorem** (vN 1929)
  $\tau = \sum_E \mathrm{Tr}(\rho\Pi_E)\frac{\Pi_E}{\mathrm{Tr}\,\Pi_E}$ mixture of microcanonical shells (a coarse version of $\overline{\rho}$).
  M = anything coarser than "quantum phase cells" (ie. coarser than some M' that commutes with the Π_E)
  What vN calls $S(\mathbf{U}_\psi) - S(\psi)$ is equal to our $D_M(\rho\|\tau)$.

  Thus von Neumann's H-theorem is of the form

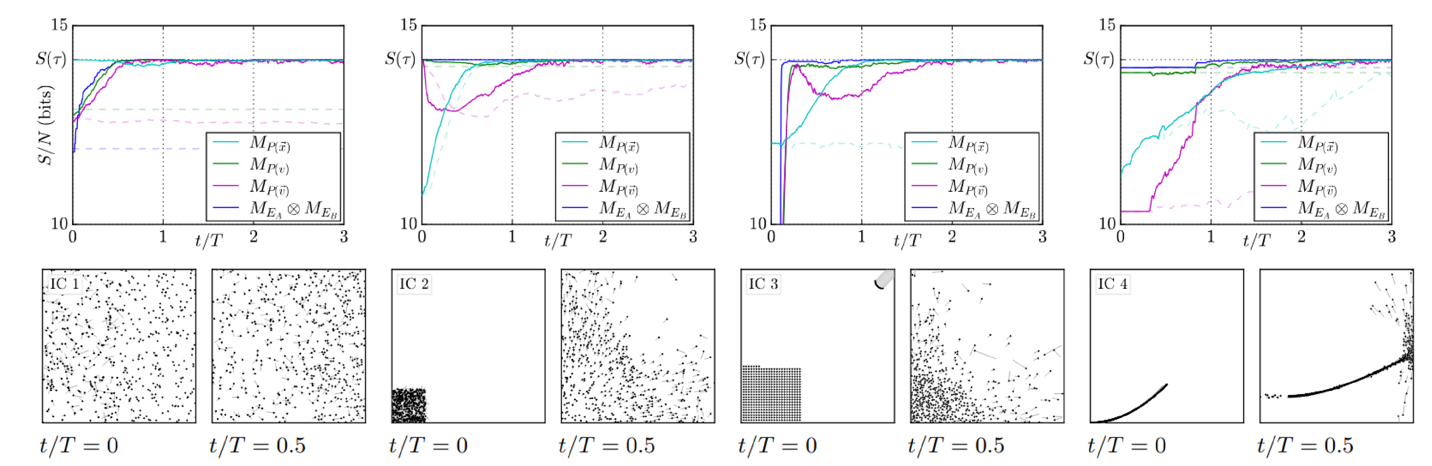
  $$S(\tau) - \overline{S_M^\tau(\rho)} \le \epsilon$$

  of same form as our main equilibration theorems (Sec. VII).



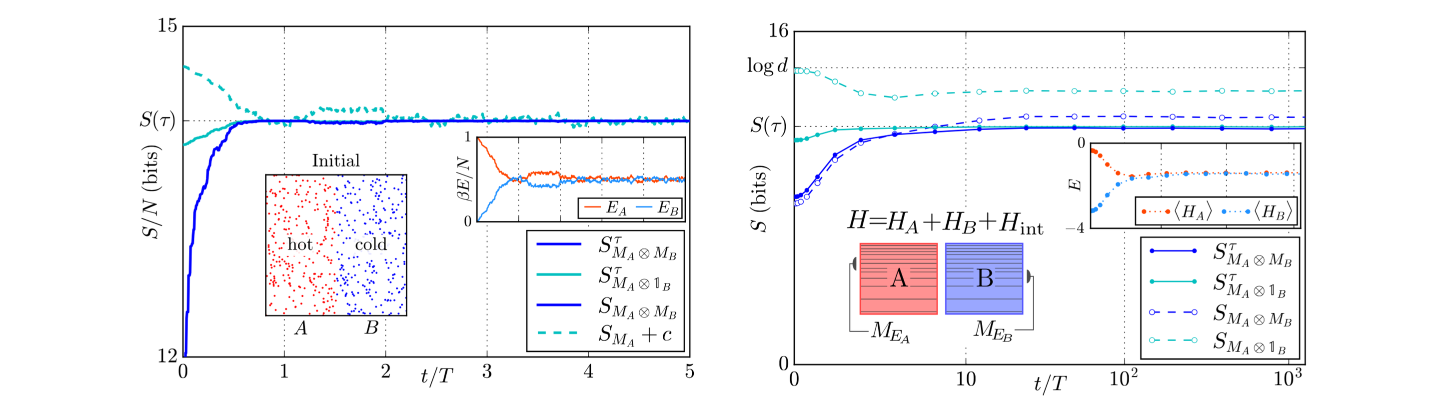
Physical Examples

Different M capture different ways a state can be low entropy!



(Depicted: Prior $\tau = e^{-\beta H}/Z$, Measurement M = spatial, velocity, speeds, or thermodynamic.)

Heat exchange in a classical hard sphere gas versus quantum random matrix model.



(Depicted: Prior $\tau = e^{-\beta H}/Z$, Measurement M = coarse local energy measurements.)

Standard thermo = energy measurements/constraints on weakly coupled subsystems. Many second laws are important: mixing the pancakes versus letting them cool.

Second Laws and Thermodynamics

In the paper we show various entropy increase theorems that can be rigorously proved for $S_M^\tau(\rho)$ in both isolated and open systems, and discuss how these entropy increase theorems connect to thermodynamics. See paper.

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