Equivalence of ensembles for general systems

Hugo Touchette

School of Mathematical Sciences
Queen Mary, University of London

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Outline

Microcanonical vs canonical

- N-particle system
- Hamiltonian: $H(\omega)$
- Macrostate: $M(\omega)$

Microcanonical $u = H/N$ — ME

$$P^u(\omega) = \text{const} \cdot \delta_{\Lambda|u}$$

- Density of states:

$$\Omega(u) = \int \delta(H(\omega) - uN)\, d\omega$$

- Entropy:

$$s(u) = \lim_{N\to\infty} \frac{1}{N} \ln \Omega(u)$$

- Equilibrium states:

$$\mathcal{E}^u = \{m^u\}$$

Canonical β — CE

$$P_\beta(\omega) = e^{-\beta H(\omega)}/Z(\beta)$$

- Partition function:

$$Z(\beta) = \int e^{-\beta H(\omega)}\, d\omega$$

- Free energy:

$$\varphi(\beta) = \lim_{N\to\infty} -\frac{1}{N} \ln Z(\beta)$$

- Equilibrium states:

$$\mathcal{E}_\beta = \{m_\beta\}$$

Equivalence of ensembles

$$\text{ME} \overset{?}{=} \text{CE}$$

Thermodynamic level

$$u \overset{?}{\longleftrightarrow} \beta$$
$$s(u) \overset{?}{\longleftrightarrow} \varphi(\beta)$$

Macrostate level

$$\mathcal{E}^u \overset{?}{\longleftrightarrow} \mathcal{E}_\beta$$

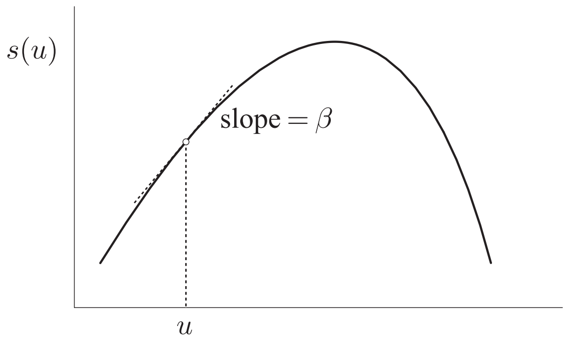
Thermo equivalence $\overset{?}{\longleftrightarrow}$ Macrostate equivalence

Main result

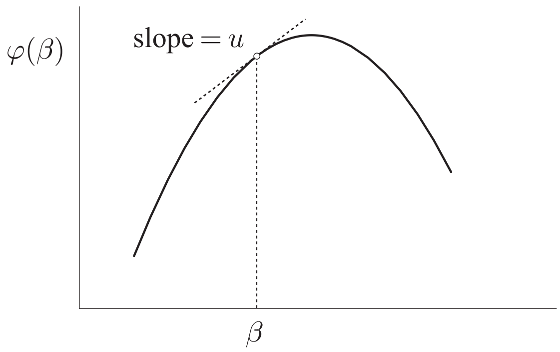
- Short-range systems have equivalent ensembles
- Long-range systems may have nonequivalent ensembles
- Related to concavity of $s(u)$

Thermodynamic equivalence

Microcanonical



Canonical



$$s(u) = \inf_{\beta}\{\beta u - \varphi(\beta)\}$$

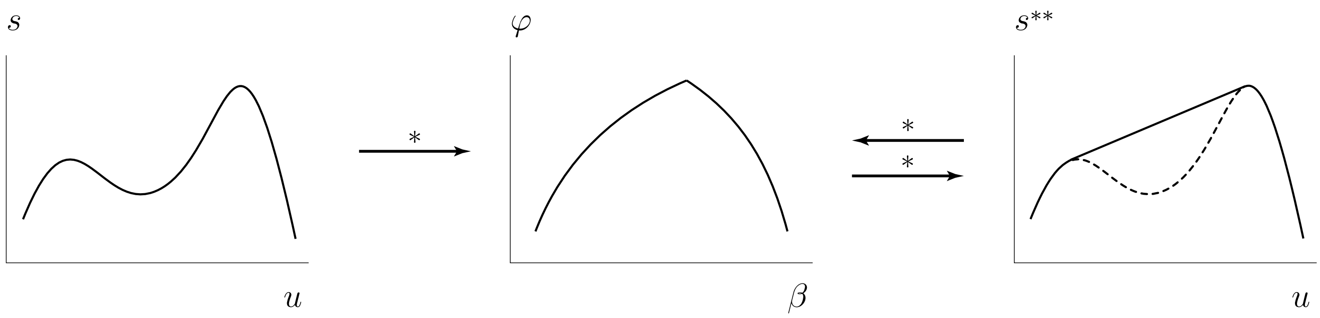
$$\varphi(\beta) = \inf_{u}\{\beta u - s(u)\}$$

$$s \longleftrightarrow \varphi$$
$$u \longleftrightarrow \beta$$

$$s = \varphi^*$$

$$\varphi = s^*$$

Thermodynamic nonequivalence



Nonconcave s

Always concave

$$\varphi = s^*$$

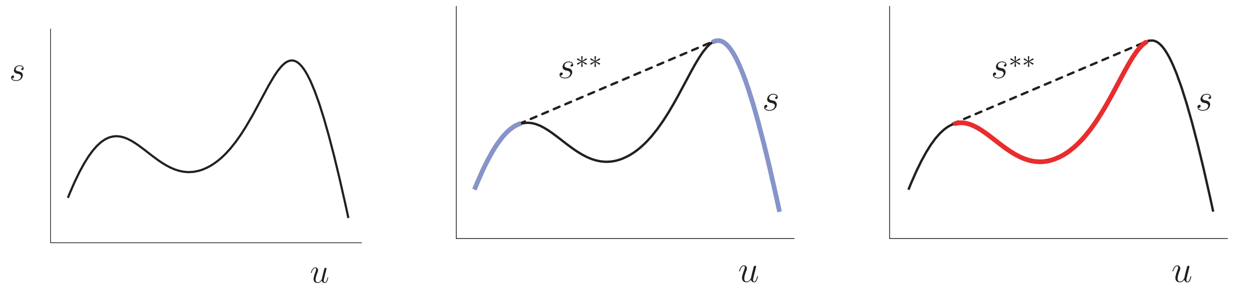
$$s \neq s^{**}$$

$$s^{**} = \varphi^*$$

- $s^{**}(u)$ = concave envelope of $s(u)$
- Negative heat capacity: $c_{\text{micro}}(u) < 0$
- Related to first-order phase transitions

Macrostate nonequivalence

[Eyink & Spohn JSP 1993; Ellis, Haven & Turkington JSP 2000]



Thermo level	$s = \varphi^*$	$s \neq \varphi^*$
Macrostate level	$\mathcal{E}^u = \mathcal{E}_\beta$	$\mathcal{E}^u \neq \mathcal{E}_\beta$

Macrostate equivalence of ensembles

[Ellis, Haven & Turkington JSP 2000]

Theorem

1. **Equivalence:**
   s strictly concave at $u \Rightarrow \mathcal{E}^u = \mathcal{E}_\beta$ for some $\beta \in \mathbb{R}$
2. **Nonequivalence:**
   s nonconcave at $u \Rightarrow \mathcal{E}^u \neq \mathcal{E}_\beta$ for all $\beta \in \mathbb{R}$
3. **Partial equivalence:**
   s concave (not strictly) at $u \Rightarrow \mathcal{E}^u \subseteq \mathcal{E}_\beta$

Assumptions

1. $H(\omega)$ can be expressed as a function of $M(\omega)$
   - Energy representation function $\tilde{h}(m)$
2. Entropy $\tilde{s}(m)$ for $M(\omega)$:
   - $s(u) = \sup_{\{m:\tilde{h}(m)=u\}} \tilde{s}(m)$

Applications

[Campa, Dauxois & Ruffo Phys Rep 2009]

Covered

- Mean field BEG model
- Mean-field Potts model
- Mean-field ϕ^4 model
- 1D α-Ising model
- Free electron laser (HMF)
- 2D point-vortex models (turbulence)

Not covered

- Gravitational systems
- Coulomb systems
- Short-range systems
- Short/long-range systems

Step 1: Equilibrium large deviations

[Lanford 1973; Ellis 1985; HT Phys Rep 2009]

Microcanonical

- Large deviation principle:

$$P^u(m) \asymp e^{-NI^u(m)}$$

- Rate function:

$$I^u(m) = \lim_{N\to\infty} -\frac{1}{N} \ln P^u(m)$$

- Equilibrium states:

$$\mathcal{E}^u = \{m : I^u(m) = 0\}$$

Canonical

- Large deviation principle:

$$P_\beta(m) \asymp e^{-NI_\beta(m)}$$

- Rate function:

$$I_\beta(m) = \lim_{N\to\infty} -\frac{1}{N} \ln P_{N,\beta}(m)$$

- Equilibrium states:

$$\mathcal{E}_\beta = \{m : I_\beta(m) = 0\}$$

Step 2: Energy decomposition of CE

CE = mixture of MEs

$$P_\beta(\omega) = \frac{e^{-\beta H(\omega)}}{Z(\beta)}, \qquad P^u(\omega) = \text{const} \cdot \delta_{\Lambda|u}$$

- Energy conditioning:
$$P_\beta(\omega|u) = P^u(\omega)$$
- Energy decomposition:
$$P_\beta(\omega) = \int P_\beta(\omega|u) P_\beta(u)\, du = \int P^u(\omega) P_\beta(u)\, du$$
- Energy LDP:
$$P_\beta(u) \asymp e^{-N J_\beta(u)}, \qquad J_\beta(u) = \beta u - s(u) - \varphi(\beta)$$
- Equilibrium energy:
$$\mathcal{U}_\beta = \{u : J_\beta(u) = 0\}$$

Step 3: Representation formula

Theorem

$$I_\beta(m) = \inf_u \{J_\beta(u) + I^u(m)\}$$

Proof:

$$\begin{aligned} P_\beta(m) &= \int P_\beta(m|u) P_\beta(u)\, du \\ &= \int P^u(m) P_\beta(u)\, du \\ &\asymp \int e^{-N[I^u(m) + J_\beta(u)]}\, du \\ &\asymp e^{-N \inf_u \{J_\beta(u) + I^u(m)\}} \end{aligned}$$

- Max of $P_\beta(m)$ = max of $P^u(m)$ and $P_\beta(u)$
- Min of $I_\beta(m)$ = min of $I^u(m)$ and $J_\beta(u)$

Main result

Assumption

- LDPs for $P_\beta(m)$ and $P^u(m)$ $\Rightarrow \begin{cases} I^u(m), I_\beta(m) \text{ exist} \\ \mathcal{E}^u, \mathcal{E}_\beta \text{ exist} \\ s(u), \varphi(\beta) \text{ exist} \end{cases}$

Theorem

1. **Equivalence:**
   $s(u)$ strictly concave $\Rightarrow \mathcal{E}^u = \mathcal{E}_\beta$ for some $\beta \in \mathbb{R}$
2. **Nonequivalence:**
   $s(u)$ nonconcave $\Rightarrow \mathcal{E}^u \neq \mathcal{E}_\beta$ for all $\beta \in \mathbb{R}$
3. **Partial equivalence:**
   $s(u)$ concave (not strictly) $\Rightarrow \mathcal{E}^u \subseteq \mathcal{E}_\beta$

Proof

$$I_\beta(m) = \inf_u \{J_\beta(u) + I^u(m)\} \qquad \begin{aligned} \mathcal{E}^u &= \{m : I^u(m) = 0\} \\ \mathcal{E}_\beta &= \{m : I_\beta(m) = 0\} \\ \mathcal{U}_\beta &= \{u : J_\beta(u) = 0\} \end{aligned}$$

- Rate functions are positive
- $I_\beta = 0$ iff $J_\beta = I^u = 0$
- $I_\beta(\mathcal{E}^{u_\beta}) = 0$

$$I_\beta(\mathcal{E}^u) = \inf_u \{J_\beta(u) + \underbrace{I^u(\mathcal{E}^u)}_{=0}\}$$

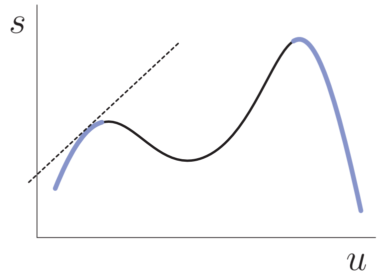
- $I^{u_\beta}(m_\beta) = 0$

$$\underbrace{I_\beta(m_\beta)}_{=0} = \inf_u \{J_\beta(u) + I^u(m_\beta)\}$$

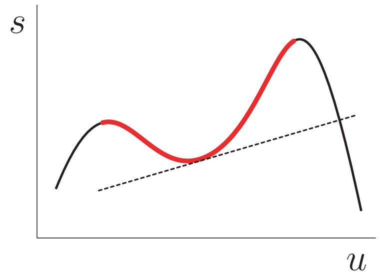
- $u \in \mathcal{U}_\beta \Leftrightarrow \beta \in \partial s(u)$

Proof (cont'd)

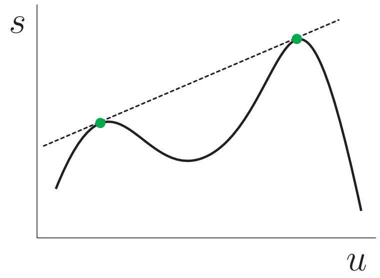
1. $s(u)$ strictly concave:
   $\Rightarrow \mathcal{U}_\beta = \{u\}$ for $\beta \in \partial s(u)$
   $\Rightarrow \mathcal{E}_\beta = \mathcal{E}^u$



2. $s(u)$ nonconcave:
   $\Rightarrow u \notin \mathcal{U}_\beta$ for any $\beta \in \mathbb{R}$
   $\Rightarrow \mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in \mathbb{R}$



3. $s(u)$ concave but not strictly:
   $\Rightarrow \mathcal{U}_\beta = \{u, u', \ldots\}$ for $\beta = \partial s(u)$
   $\Rightarrow \mathcal{E}^u \subseteq \mathcal{E}_\beta$



Other results

Covering

$$\mathcal{E}_\beta = \bigcup_{u \in \mathcal{U}_\beta} \mathcal{E}^u$$

- $\mathcal{U}_\beta = \tilde{h}(\mathcal{E}_\beta)$ if $\tilde{h}$ exists
- $\tilde{h}$ and $\tilde{s} \rightarrow I^u$ and I_β
- I^u and I_β exist without $\tilde{h}$ and $\tilde{s}$

- [Ellis, Haven & Turkington JSP 2000]:

$$\mathcal{E}_\beta = \bigcup_{u \in \tilde{h}(\mathcal{E}_\beta)} \mathcal{E}^u$$

Phase coexistence

$$s(u) \text{ nonconcave or affine} \Leftrightarrow \mathcal{E}_\beta = \mathcal{E}^u \cup \mathcal{E}^{u'} \cup \cdots$$

Systems now covered

- Non-mean-field systems
- Long-range systems
- Gravitating systems
- Short-range systems
- Mixed short/long-range systems
- Macrostates with no energy representation functions
- Many macrostates for given model
- ...

Example 1: 1D α-Ising model

[Barré, Bouchet, Dauxois & Ruffo JSP 2005; Dyson CMP 1969]

- 1D spin model:

$$H = \frac{J}{N^{1-\alpha}} \sum_{i>j=1}^{N} \frac{1 - S_i S_j}{|i-j|^\alpha}, \qquad J > 0, S_i = \pm 1$$

- Mean-field limit for $0 \leq \alpha < 1$
- "Mean-field" macrostate: Magnetization profile $m(x)$
- Standard magnetization:

$$M = \frac{1}{N} \sum_{i=1}^{N} S_i$$

- No energy representation function for M
- Entropy $s(u)$ is known
- Equivalence (either strict or partial)

Example 2: Short/long-range models

[Campa, Giansanti, Mukamel & Ruffo Physica 2006]

- Coupled rotators (generalized HMF):

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \underbrace{\frac{J}{2N} \sum_{i,j=1}^{N} [1 - \cos(\theta_i - \theta_j)]}_{\text{Long-range}} - \underbrace{K \sum_{i=1}^{N} \cos(\theta_{i+1} - \theta_i)}_{\text{Short-range}}$$

- Macrostate:

$$M = \frac{1}{N} \sqrt{\left(\sum_{i=1}^{N} \cos\theta_i\right)^2 + \left(\sum_{i=1}^{N} \sin\theta_i\right)^2}$$

- No representation function for M
- Entropy $s(u)$ is known
- Nonequivalence for $-0.25 < K < K_1 \approx -0.168$

Example 3: 2D Ising model

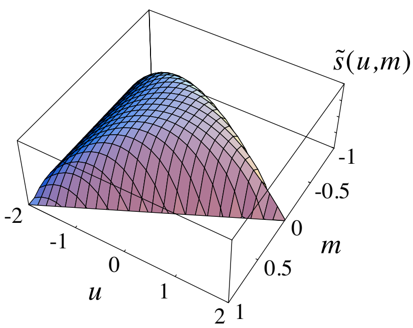
- Hamiltonian:

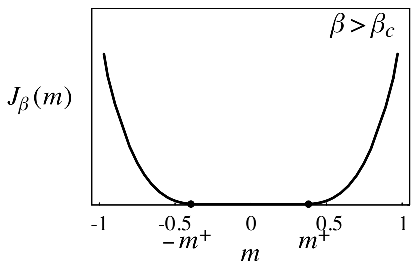
$$H_N = -\frac{1}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \qquad \sigma_i = \pm 1$$

- Magnetization: $M = \frac{1}{N} \sum_i \sigma_i$
- No energy representation function
- Entropy $s(u, m)$ is known
- Equivalence for strictly concave parts
- Problems for flat parts
- Bulk + surface LDPs:

$$P(m) \asymp e^{-NJ(m) - \sqrt{N} I(m)}$$

- Equivalence determined by bulk + surface





Conclusions

Thermodynamic equivalence $\Leftrightarrow$ Macrostate equivalence

- General result of statistical mechanics

Covers:

- Any (classical) many-body system
- Any (valid) macrostate
- Canonical / Grand-canonical
- Any other dual ensembles
- Higher-dimensional Hamiltonian / macrostates
  - e.g., turbulence models: $H = \{\text{energy, circulation}\}$
- Nonequilibrium particle models (e.g., zero-range process)

Future work:

- Include surface LDPs
- Relative entropy equivalence: $H(P_\beta | P^u) = 0$
- Quantum systems

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