Long-range systems with nonequivalent ensembles

Hugo Touchette

National Institute for Theoretical Physics (NITheP)
Stellenbosch, South Africa

Long-range interacting many-body systems
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Outline

1. Statistical ensembles
2. Thermodynamic equivalence
3. Macrostate equivalence
4. Microstate equivalence
5. Examples

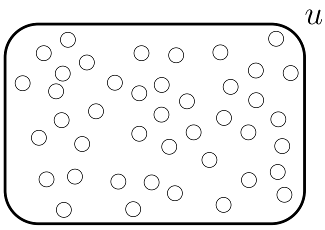
Thermodynamic	$F = E - TS$
Macrostates	$M(\omega)$
Microstates	$\omega = (\omega_1, \ldots, \omega_N)$

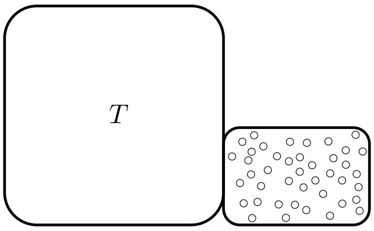
Referee B

Ensemble inequivalence is not important, since systems with long-range forces do not evolve to equilibrium

Equilibrium statistical mechanics

- N-particle system
- Microstate: $\omega = (\omega_1, \ldots, \omega_N)$
- Hamiltonian: $H(\omega)$
- Macrostate: $M(\omega)$
- Ensemble: $P^u(\omega)$ or $P_\beta(\omega)$
- Closed or open system





- Thermodynamic functions: $s(u)$, $f(\beta)$
- Equilibrium states
- Control parameters: u or β

Statistical ensembles

Microcanonical ME

- Parameter: $u = H/N$
- Microstate distribution:

$$P^u(\omega) = \begin{cases} \text{const} & H(\omega)/N = u \\ 0 & \text{otherwise} \end{cases}$$

- 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 CE

- Parameter: $\beta = (k_B T)^{-1}$
- Microstate distribution:

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

- Partition function:

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

- Free energy:

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

- Equilibrium states: $\mathcal{E}_\beta = \{m_\beta\}$

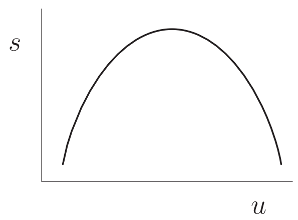
Equivalence of ensembles

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

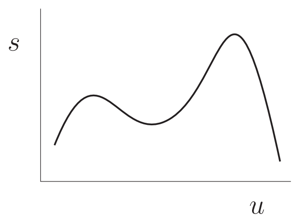
Thermodynamic	Macrostate	Measure
$u \stackrel{?}{\longleftrightarrow} \beta$ $s(u) \stackrel{?}{\longleftrightarrow} \varphi(\beta)$	$\mathcal{E}^u \stackrel{?}{\longleftrightarrow} \mathcal{E}_\beta$	$P^u \stackrel{?}{\longleftrightarrow} P_\beta$

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

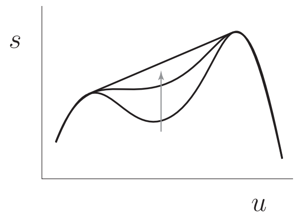
Short-range



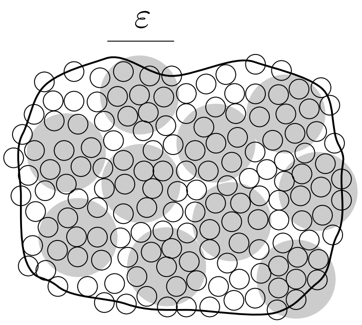
Long-range

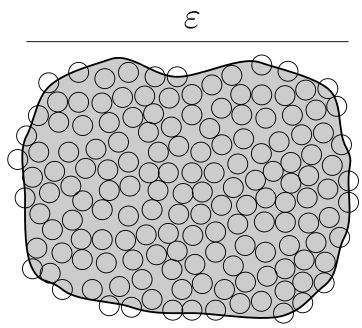


Small (finite)



Short- vs long-range interactions





- Finite-range interaction
- Finite correlation length
- Extensive energy: $U \sim N$
- Bulk dominates over surface
- Sub-system separation
- Entropy always concave

- Interaction is ‘infinite’ range
- Infinite correlation length
- Non-extensive energy
- Bulk $\sim$ surface
- No separation
- Entropy possibly nonconcave

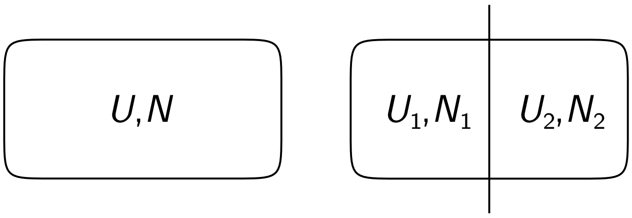
Thermodynamics and statistical mechanics still defined

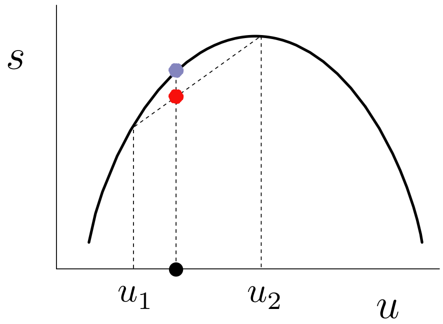
Concave entropy for short-range interactions

- Entropy:

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

- Separation argument:





$$U \approx U_1 + U_2$$

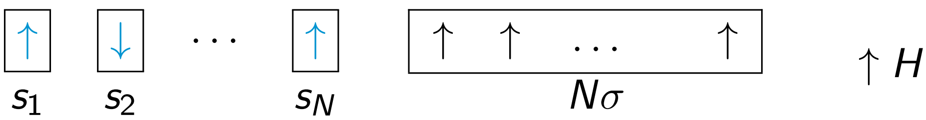
$$\Omega_N(U_1+U_2) \geq \Omega_{N_1}(U_1)\,\Omega_{N_2}(U_2)$$

$$s(\alpha u_1 + \bar{\alpha} u_2) \geq \alpha s(u_1) + \bar{\alpha} s(u_2)$$

Two-block spin model [HT Am J Phys 2008]

Referee A

Entropy is always concave (at least I cannot imagine a counterexample)

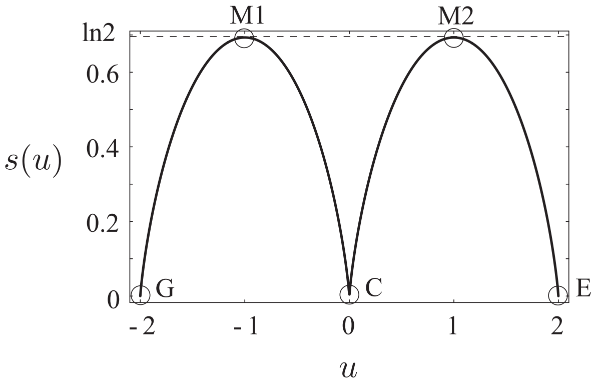


- Total energy: $U = \sum_{i=1}^{N} s_i + N\sigma$
- Energy per spin:

$$u = \frac{U}{N} \in [-2, 2]$$

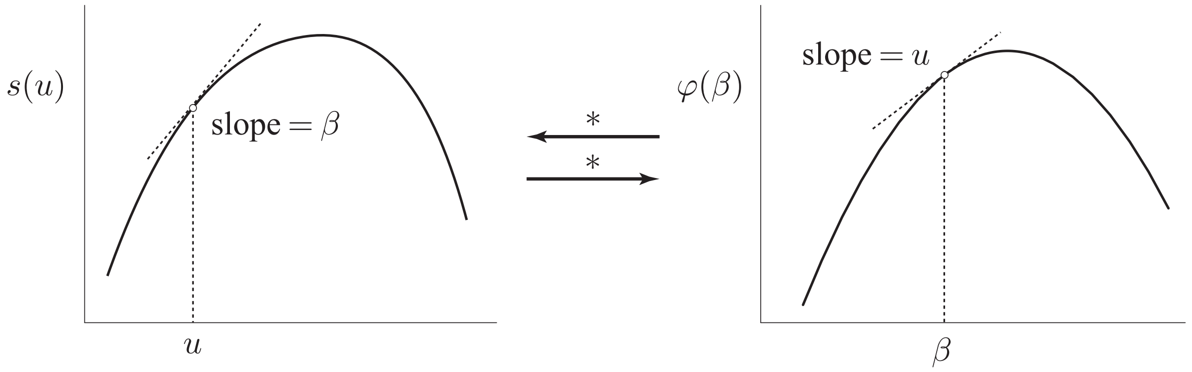
- Entropy:

$$s(u) = \begin{cases} s_0(u+1) & u \in [-2,0] \\ s_0(u-1) & u \in (0,2] \end{cases}$$



Thermodynamic equivalence

Microcanonical | **Canonical**



$$s(u) = \beta u - \varphi(\beta)$$
$$\varphi'(\beta) = u$$

$$\varphi(\beta) = \beta u - s(u)$$
$$s'(u) = \beta$$

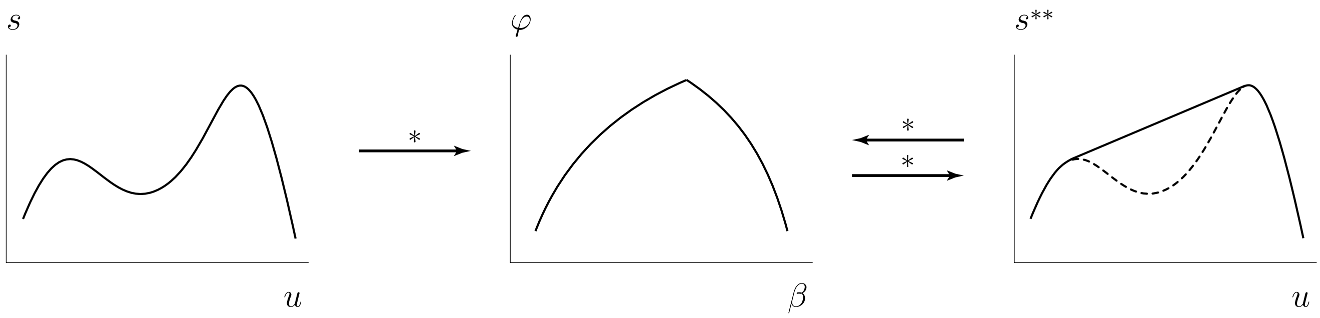
$$s \longleftrightarrow \varphi$$
$$u \longleftrightarrow \beta$$

$$s = \varphi^*$$

$$\varphi = s^*$$

Thermodynamic equivalence of ensembles

Thermodynamic nonequivalence



Non-concave

s

Always concave

$$\varphi = s^*$$

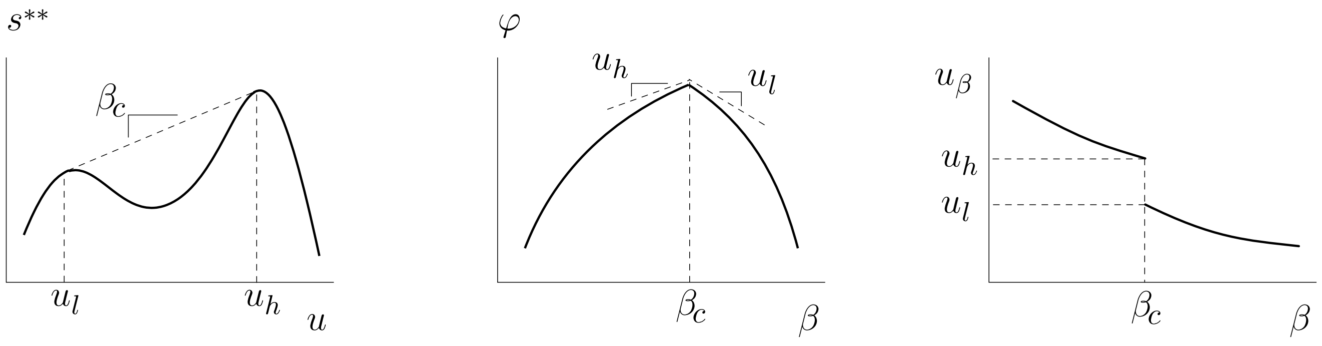
$$s \neq \varphi^* = s^{**}$$

Concave envelope

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

- Thermodynamic nonequivalence of ensembles
- Part of $s(u)$ not recovered by $\varphi(\beta)$
- Microcanonical properties not seen canonically

First-order phase transitions



- $s(u)$ nonconcave $\Rightarrow \varphi(\beta)$ non-differentiable
- First-order phase transition in canonical ensemble
- Latent heat: $\Delta u = u_h - u_l$
- Canonical skips over microcanonical

Macrostate equivalence

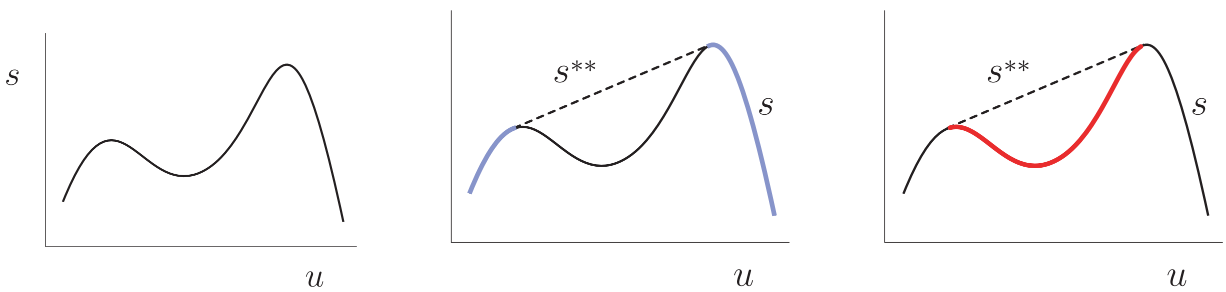
Thermo	$u \leftrightarrow \beta$
Macro	$M_N(\omega)$
Micro	$(\omega_1, \ldots, \omega_N)$

Microcanonical

- $P^u(M_N = m)$
- $\mathcal{E}^u = \{m^*\}$

Canonical

- $P_\beta(M_N = m)$
- $\mathcal{E}_\beta = \{m^*\}$



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

Mean-field Potts model

[Costeniuc, Ellis & HT JMP 2005]

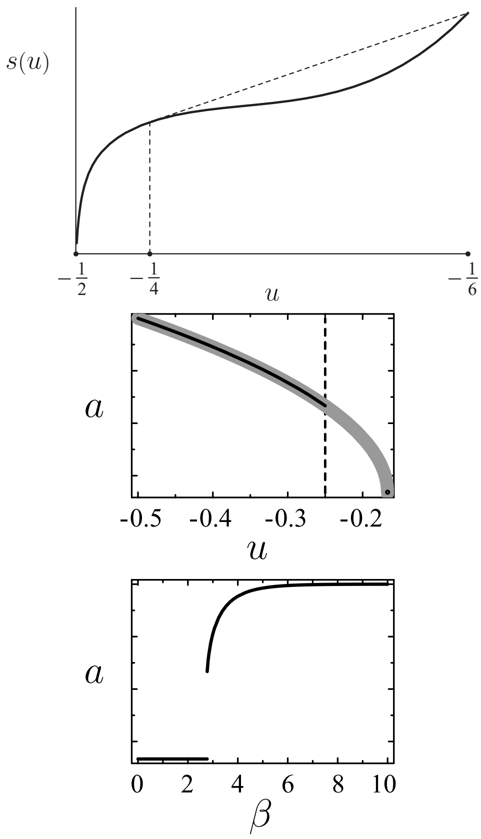
- Hamiltonian:

$$H = -\frac{1}{2N}\sum_{i,j=1}^{N}\delta_{\omega_i,\omega_j}, \quad \omega_i \in \{1,2,3\}$$

- Distribution of spins: $\nu = (a, b, b)$
- Macrostate:

$$a = \frac{\#\text{ spins } 1}{N}$$

  - ME macrostate: $a(u)$
  - CE macrostate: $a(\beta)$
- Nonconcave entropy
  - Nonequivalent ensembles
  - First-order canonical phase transition
  - Metastable states



Basic idea

$$P_\beta(\omega) = \frac{e^{-\beta H(\omega)}}{Z(\beta)}, \qquad P^u(\omega) = \begin{cases} \text{const} & H(\omega)/N = u \\ 0 & \text{otherwise} \end{cases}$$

1. Canonical with fixed energy = microcanonical

$$P_\beta(\omega|u) = P^u(\omega)$$

2. Canonical = mixture of microcanonical

$$\underbrace{P_\beta(m)}_{\text{CE}} = \underbrace{\int P_\beta(m|u)\, P_\beta(u)\, du}_{\text{Bayes Theorem}} = \int \underbrace{P^u(m)}_{\text{ME}}\, P_\beta(u)\, du$$

3. Consequence:

$$\mathcal{E}_\beta = \bigcup_{\underbrace{u\in\mathcal{U}_\beta}_{\text{Equilibrium energies}}} \mathcal{E}^u$$

4. $\mathcal{U}_\beta$ determined by concavity of $s(u)$

Measure equivalence

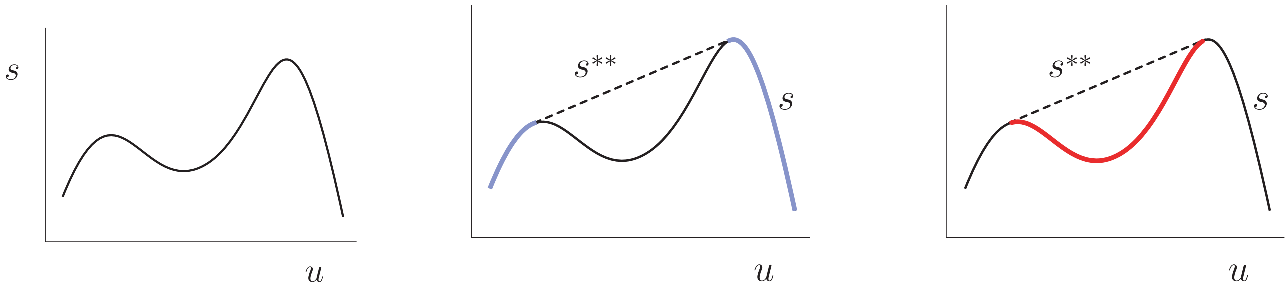
- Microstate: $\omega = (\omega_1, \dots, \omega_N)$

Microcanonical

$$P^u(\omega) = \begin{cases} \text{const} & H(\omega)/N = u \\ 0 & \text{otherwise} \end{cases}$$

Canonical

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



$$\lim_{N\to\infty} \frac{1}{N} \ln \frac{P^u(\omega)}{P_\beta(\omega)} = 0$$

$$\lim_{N\to\infty} \frac{1}{N} \ln \frac{P^u(\omega)}{P_\beta(\omega)} \neq 0$$

- $P^u(\omega) \approx P_\beta(\omega)$
- For almost all microstates

Recap

Thermodynamic	$s \leftrightarrow \varphi$ $u \leftrightarrow \beta$	
Macrostates	$\mathcal{E}^u = \mathcal{E}_\beta$	$s'(u) = \beta$
Microstates	$P^u(\omega) \approx P_\beta(\omega)$	

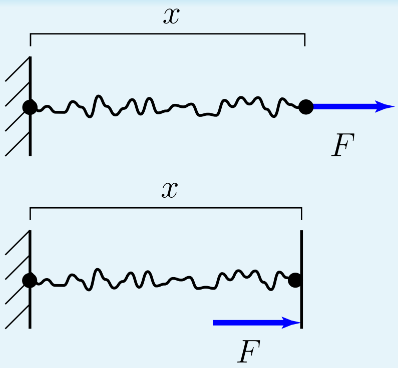
- Equivalence: $s(u)$ concave
- Nonequivalence: $s(u)$ nonconcave
- Valid for any macrostate
- Energy constraint can be replaced by other constraints

Other ensembles

Stretching

[Cluzel et al Science 1996, Sinha & Samuel PRE 2005]

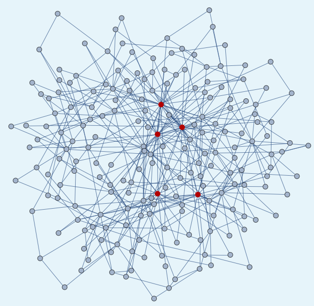
- Isotensional ensemble:
  - $F = \text{const}$
  - x fluctuates
- Isometric ensemble:
  - $x = \text{const}$
  - F fluctuates



Graphs

[Squartini et al PRL 2015]

- Ensemble of graphs: $P(G)$
- Fixed node number
- Fixed degree sequence: $\{k_1, k_2, \ldots\}$
- Fixed distribution of degrees



Generalized ensembles

[Costeniuc, Ellis, HT & Turkington JSP 2005]

Canonical ensemble

$$Z(\beta) = \sum_\omega e^{-\beta U}$$

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

$$s \neq \varphi^*$$

Generalized canonical ensemble

$$Z_g(\beta) = \sum_\omega e^{-\beta U - N g(U/N)}$$

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

$$s = {\varphi_g}^* + g$$

- Recover equivalence with modified Legendre transform
- Gaussian ensemble: $g(u) = \gamma u^2$
- Betrag ensemble: $g(u) = \gamma |u - u_0|$
- Universal ensembles: equivalence recovered with $\gamma \to \infty$

Conclusion

Fixed constraint	Average constraint
$P(\omega \| H = u)$	$Q(\omega) = e^{-\beta H(\omega)}$
Conditioning (micro)	Exponential tilting (cano)

- Asymptotic equivalence of distributions
- Many Q equivalent to P

More physical problems

- What interactions lead to nonequivalent ensembles?
- Can we experimentally measure nonconcave entropies?

References

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