Relationships of Solutions of Constrained and Unconstrained Minimization Problems with Applications to Nonequivalence of Ensembles in Statistical Mechanics

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Mathematical Motivation

- $\mathcal{X}$ a complete, separable metric space
- I a rate function on $\mathcal{X}$: l.s.c., compact level sets, $I : \mathcal{X} \to [0, \infty]$
- f bounded and continuous, $f : \mathcal{X} \to \mathbb{R}$

Mathematical core of this talk: investigate the relationships between the solutions of the following two minimization problems.

1. Minimization with a constraint for u given:

$$\text{Minimize } I(\nu) \text{ over } \mathcal{X} \text{ subject to } f(\nu) = u.$$

2. Dual minimization without a constraint for β given:

$$\text{Minimize } I(\nu) + \beta f(\nu) \text{ over } \mathcal{X}.$$

Main results

- Problems 1. and 2. express the asymptotic behavior of the microcanonical ensemble and the canonical ensemble. Derive via large deviations.
- There are only **three** possible relationships between solutions of 1. and 2. These relationships are expressed by concavity properties of the microcanonical entropy

$$s(u) \doteq -\inf\{I(\nu) \colon \nu \in \mathcal{X}, f(\nu) = u\}.$$

Physical Motivation

Two choices of probability distributions in equilibrium statistical mechanics:

Microcanonical ensemble
$u = \text{const}$

$$\uparrow \; ? \; \downarrow$$

Canonical ensemble
β or $T = \text{const}$

- Are the two probability distributions equivalent?
- Equivalence of ensembles:
  - Example: perfect gas
  - General conditions: short-range interactions
- Nonequivalence of ensembles:
  - Example: before the thermodynamic limit
  - Examples in the thermodynamic limit
    - Models of fluid and geostrophic turbulence
    - Lattice spin systems
  - General conditions: long-range interactions?
  - Physical consequences for observables?

■ Outline of talk

- Statistical mechanical ensembles: short review
- Large deviation methodology
- Thermodynamic nonequivalence
  - At level of microcanonical entropy and canonical free energy per particle
- Macrostate nonequivalence
  - At level of microcanonical and canonical equilibrium macrostates
- Comments on models of turbulence
  - Use statistical theories to predict the formation, interaction, and stability of large-scale, coherent structures; e.g., vorticies and shears in fluid motion, Earth ocean waves, the Great Red Spot of Jupiter, solitons.
- Illustration of results: mean-field Blume-Emery-Griffiths spin model
- Relationship with phase transitions
- Conclusion
- Bibliography

Statistical mechanical ensembles

Boltzmann (1872), Gibbs (1876, 1902)

- ω_i, $i = 1, 2, \ldots, n$, each $\omega_i \in \Lambda$ (spins or vorticities or ...)
- Microstates: $\omega \doteq (\omega_1, \omega_2, \ldots, \omega_n) \in \Lambda^n$
- Hamiltonian or energy function: $H_n(\omega)$
- Energy per particle: $h_n(\omega) \doteq \frac{1}{n} H_n(\omega)$
- A priori measure P_n; e.g., if Λ is a finite set,

$$P_n(\{\omega\}) \doteq \frac{1}{|\Lambda|^n} \text{ for each } \omega$$

- Macroscopic variable $L_n(\omega)$ bridging microscopic and macroscopic descriptions: $L_n(\omega)$ maps Λ^n into a space $\mathcal{X}$ ($[-1, 1]$ or $\mathcal{P}(\Lambda)$ or $L^2(\Lambda)$ or ...).
  - $\mathcal{X}$ is space of macrostates.
  - Require bounded, continuous energy representation function f mapping $\mathcal{X}$ into $\mathbb{R}$: as $n \to \infty$

$$h_n(\omega) = f(L_n(\omega)) + \mathrm{o}(1) \text{ uniformly over } \omega.$$

  - Require basic LDP with respect to P_n:

$$P_n\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI(\nu)},$$

  $I(\nu)$ rate function for macrostates $\nu \in \mathcal{X}$.

□ Example: Curie-Weiss spin model

- n spins $\omega_i \in \{-1, 1\}$
- Microstates: $\omega \doteq (\omega_1, \omega_2, \ldots, \omega_n) \in \{-1, 1\}^n$
- Hamiltonian:

$$H_n(\omega) \doteq -\frac{1}{2n} \underbrace{\left(\sum_{i=1}^n \omega_i\right)^2}_{\text{magnetization}}$$

- Energy per particle:

$$h_n(\omega) \doteq -\frac{1}{n} H_n(\omega) = -\frac{1}{2} \underbrace{\left(\frac{1}{n} \sum_{i=1}^n \omega_i\right)^2}_{\text{magn. per part.}}$$

- A priori measure:

$$P_n(\{\omega\}) \doteq \frac{1}{2^n} \text{ for each } \omega$$

- Macroscopic variable:

$$L_n(\omega) \doteq \frac{1}{n} \sum_{i=1}^n \omega_i \in [-1, 1]$$

  - Energy representation function f:

$$h_n(\omega) = f(L_n(\omega)), \;\; f(\nu) \doteq -\tfrac{1}{2}\nu^2 \text{ for } \nu \in [-1, 1]$$

  - Basic LDP:

Cramér's Theorem: $P_n\Big\{\omega : \frac{1}{n} \sum_{i=1}^n \omega_i \approx \nu\Big\} \asymp e^{-nI(\nu)}$,

$$I(\nu) \doteq \frac{1-\nu}{2} \log(1-\nu) + \frac{1+\nu}{2} \log(1+\nu) \text{ for } \nu \in [-1, 1]$$

□ Models to which formalism has been applied

- Miller-Robert model of fluid turbulence based on the 2D Euler equations
- Model of geophysical flows based on equations describing barotropic, quasi-geostrophic turbulence
- Model of soliton turbulence based on a class of generalized nonlinear Schrödinger equations
- Q-state Curie-Weiss-Potts spin model
- Mean-field Blume-Emery-Griffiths spin model

- A priori measure: $P_n(\{\omega\}) \doteq \frac{1}{|\Lambda|^n}$ for each $\omega \in \Lambda^n$
- Assumption: $L_n(\omega)$ maps Λ^n into $\mathcal{X}$ such that
  - $h_n(\omega) = f(L_n(\omega)) + \text{o}(1)$ for bdd. cont. $f\colon \mathcal{X} \to \mathbb{R}$
  - $\exists$ rate function $I(\nu)$ for macrostates $\nu \in \mathcal{X}$:

$$P_n\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI(\nu)}$$

□ Microcanonical ensemble P_n^u

$$P_n^u(d\omega) \doteq P_n(d\omega \mid h_n(\omega) \approx u)$$

- Postulate of equiprobability. If Λ is a finite set and $P_n(\{\omega\}) = \frac{1}{|\Lambda|^n}$ for each ω, then the conditional probability P_n^u is constant on energy shell $\{\omega : h_n(\omega) \approx u\}$.

- Microcanonical entropy $s(u)$:

$$\boxed{P_n\{\omega : h_n(\omega) \approx u\} \asymp e^{ns(u)}, \;\; s(u) \doteq -\inf\{I(\nu) : f(\nu) = u\}}$$

$$\begin{aligned} P_n\{\omega : h_n(\omega) \approx u\} &\approx P_n\{\omega : f(L_n(\omega)) \approx u\} \\ &= P_n\{\omega : L_n(\omega) \in f^{-1}(u)\} \\ &\asymp \sup\big\{\exp[-nI(\nu) : \nu \in f^{-1}(u)]\big\} \\ &= \exp[-n \cdot \inf\{I(\nu) : \nu \in f^{-1}(u)\}] \\ &= \exp[-n \cdot \underbrace{\inf\{I(\nu) : f(\nu) = u\}}_{-s(u)}] \end{aligned}$$

- Asymptotic P_n^u-distribution for $L_n(\omega)$:

If $\nu \in \mathcal{X}$ satisfies $f(\nu) = u$, then

$$\begin{aligned} & P_n^u\{\omega : L_n(\omega) \approx \nu\} \\ & = P_n\{\omega : L_n(\omega) \approx \nu, h_n(\omega) \approx u\} \cdot \frac{1}{P_n\{\omega : h_n(\omega) \approx u\}} \\ & \approx P_n\{\omega : L_n(\omega) \approx \nu, f(L_n(\omega)) \approx u\} \cdot \frac{1}{P_n\{\omega : h_n(\omega) \approx u\}} \\ & = P_n\{\omega : L_n(\omega) \approx \nu\} \cdot \frac{1}{P_n\{\omega : h_n(\omega) \approx u\}} \\ & \asymp \exp[-n(I(\nu) + s(u))]. \end{aligned}$$

If $f(\nu) \neq u$, then $P_n^u\{\omega : L_n(\omega) \approx \nu\} \asymp 0$.

- LDP for P_n^u-distribution of $L_n(\omega)$:

$$\boxed{\begin{gathered} P_n^u\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI^u(\nu)} \\ I^u(\nu) \doteq \begin{cases} I(\nu) + s(u) & \text{if } f(\nu) = u \\ \infty & \text{otherwise} \end{cases} \end{gathered}}$$

- Microcanonical equilibrium macrostates defined by $I^u(\nu) = 0$:

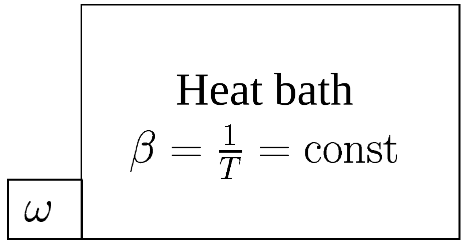
  $I^u(\nu) \geq 0$ for all ν

  $I^u(\nu) > 0 \Longrightarrow P_n^u\{\omega : L_n(\omega) \approx \nu\} \to 0$ exponentially fast

  $I^u(\nu) = 0 \Longleftrightarrow I(\nu) = -s(u) = \inf\{I(\mu) : f(\mu) = u\}$.

$$\boxed{\mathcal{E}^u = \{\nu \in \mathcal{X} : I(\nu) \text{ is minimized for } f(\nu) = u\}}$$

□ Canonical ensemble $P_{n,\beta}$



- Gibbs probability distribution:

$$P_{n,\beta}(d\omega) \doteq \frac{1}{Z_n(\beta)} e^{-\beta n h_n(\omega)} P_n(d\omega),$$
$$Z_n(\beta) \doteq \int_{\Lambda^n} e^{-\beta n h_n(\omega)} P_n(d\omega) \asymp e^{-n\varphi(\beta)}$$

$\varphi(\beta)$ is canonical free energy per particle.

- LDP for $P_{n,\beta}$-distribution of $L_n(\omega)$:

$$\boxed{\begin{array}{c} P_{n,\beta}\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI_\beta(\nu)} \\ I_\beta(\nu) \doteq I(\nu) + \beta f(\nu) - \varphi(\beta) \end{array}}$$

- Canonical equilibrium macrostates defined by $I_\beta(\nu) = 0$:

  $I_\beta(\nu) \geq 0$ for all ν

  $I_\beta(\nu) > 0 \Rightarrow P_{n,\beta}\{\omega : L_n(\omega) \approx \nu\} \to 0$ exponentially fast

$$\boxed{\mathcal{E}_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) \text{ is minimized}\}}$$

- Microcanonical equilibrium macrostates defined by $I^u(\nu) = 0$:

$$\boxed{\mathcal{E}^u = \{\nu \in \mathcal{X} : I(\nu) \text{ is minimized for } f(\nu) = u\}}$$

Nonequivalence of ensembles: thermodynamic point of view

Microcanonical entropy s	$\stackrel{?}{=}$	Legendre-Fenchel transform $\varphi^* = s^{**}$

- Canonical free energy per particle $\varphi(\beta)$:

$$Z_n(\beta) \doteq \int_{\Lambda^n} e^{-\beta n h_n(\omega)}\, P_n(d\omega) \asymp e^{-n\varphi(\beta)},$$

$$\varphi(\beta) \doteq -\lim_{n\to\infty} \frac{1}{n} \log Z_n(\beta)$$

- Free energy φ is Legendre-Fenchel transform of entropy s:

$$Z_n(\beta) = \int_{\mathbb{R}} e^{-\beta n u}\, P_n\{\omega : h_n(\omega) \in du\}$$

$$\asymp \int_{\mathbb{R}} e^{-\beta n u}\, e^{n s(u)}\, du \asymp \exp\big[-n \cdot \underbrace{\inf_u\{\beta u - s(u)\}}_{\varphi(\beta)}\big]$$

$$\boxed{\varphi(\beta) = \inf_u\{\beta u - s(u)\} \doteq s^*(\beta)}$$

- Inversion of Legendre-Fenchel transform:

$$s(u) \stackrel{?}{=} \inf_\beta\{\beta u - \varphi(\beta)\} \doteq \varphi^*(u)$$

  - Equality if $s(u)$ is concave or $\varphi(\beta)$ differentiable
    - ∗ Thermodynamic equivalence of ensembles
  - $\varphi(\beta)$ is always concave.

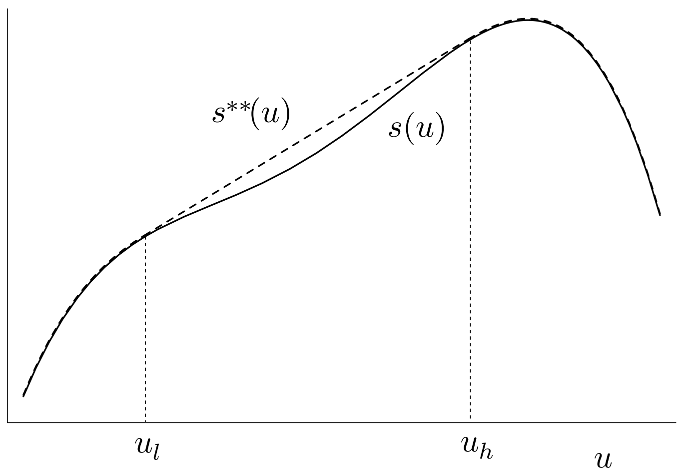
- Concave hull $s^{**}(u)$ of $s(u)$:

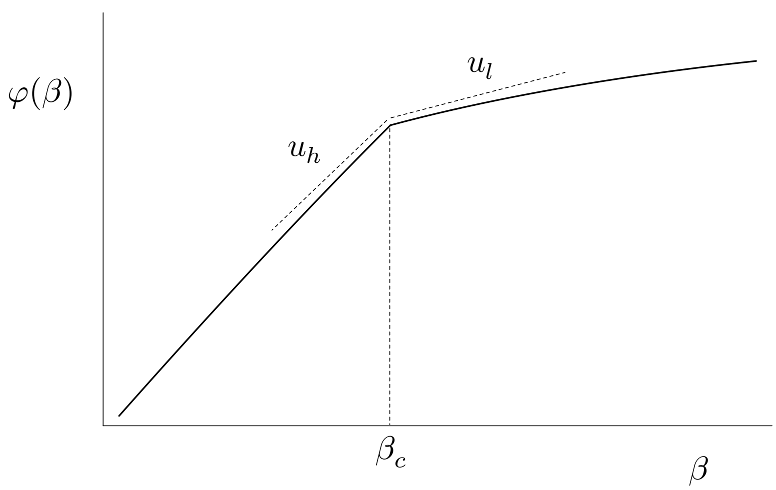
$$s^{**}(u) \doteq \inf_{\beta}\{\beta u - s^*(\beta)\} = \inf_{\beta}\{\beta u - \varphi(\beta)\}$$

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

- **Thermodynamic** nonequivalence:

$$s^{**}(u) \neq s(u)$$





□ From thermodynamic point of view, microcanonical ensemble is more basic

From $s(u)$ to $\varphi(\beta)$

- $s(u)$ was introduced as rate function in LDP

  $P_n\{\omega : h_n(\omega) \approx u\} \asymp e^{ns(u)},\ s(u) \doteq -\inf\{I(\nu) : f(\nu) = u\}.$

  This implies

  $$\varphi(\beta) \doteq -\tfrac{1}{n}\log Z_n(\beta) = \inf_u\{\beta u - s(u)\}.$$

From $\varphi(\beta)$ to $s(u)$

- Suppose one proves that $\varphi(\beta)$ exists. Calculate rate function $s(u)$ by Gärtner-Ellis Theorem. If $\varphi(\beta)$ differentiable, then

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

  By convex duality, $s(u)$ is strictly concave.

Possibilities starting from φ (complicated)

- $\varphi(\beta)$ differentiable $\Longrightarrow s(u) = \inf_\beta\{\beta u - \varphi(\beta)\}$ strictly concave

- $\varphi(\beta)$ not differentiable $\Longrightarrow$

  - EITHER $s(u) = \inf_\beta\{\beta u - \varphi(\beta)\}$ (not strictly) concave

  - OR $s(u)$ not concave, $s(u) \neq s^{**}(u) = \inf_\beta\{\beta u - \varphi(\beta)\}$

Nonequivalence of ensembles: point of view of equilibrium macrostates

Properties of microcanonical equilibrium macrostates	$\stackrel{?}{=}$	Properties of canonical equilibrium macrostates

- Microcanonical equilibrium macrostates (**minimization with constraint**):

$$\nu^u = \arg \inf_{\{\nu : f(\nu) = u\}} I(\nu)$$

Find extremal points of $I(\nu) + \beta f(\nu)$ via

$$\beta = \beta(u): \text{ Lagrange multiplier dual to } f(\nu) = u.$$

- Canonical equilibrium macrostates (**dual minimization without constraint**):

$$\nu_\beta = \arg \inf_\nu \{I(\nu) + \beta f(\nu)\}$$

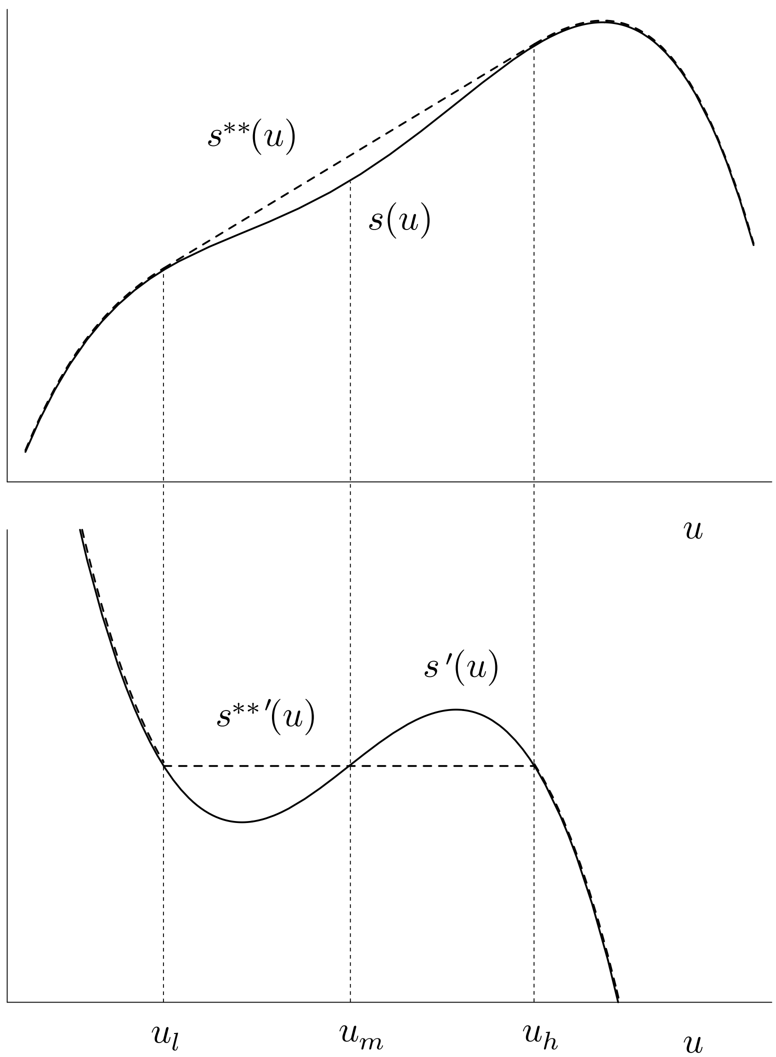
- Questions of equivalence and nonequivalence:
  - Does $\nu^u = \nu_\beta$ for u or β given?
  - Do there exist $\beta(u)$ such that $\nu^u = \nu_{\beta(u)}$ and $u(\beta)$ such that $\nu^{u(\beta)} = \nu_\beta$?
  - Max in $\varphi(\beta) = \inf_u \{\beta u - s(u)\}$ at $\beta = \beta(u) = s'(u)$
  - Unless s is strictly concave, $\beta = s'(u)$ cannot be inverted to give unique $u = u(\beta) = (s')^{-1}(\beta)$.

Thermodynamic vs. macrostate points of view

Full equivalence on the level of equilibrium macrostates

- $\Longleftrightarrow$ microcanonical entropy $s(u)$ is strictly concave.
- $\Longleftrightarrow$ canonical free energy $\varphi(\beta)$ is differentiable (absence of first-order phase transition).

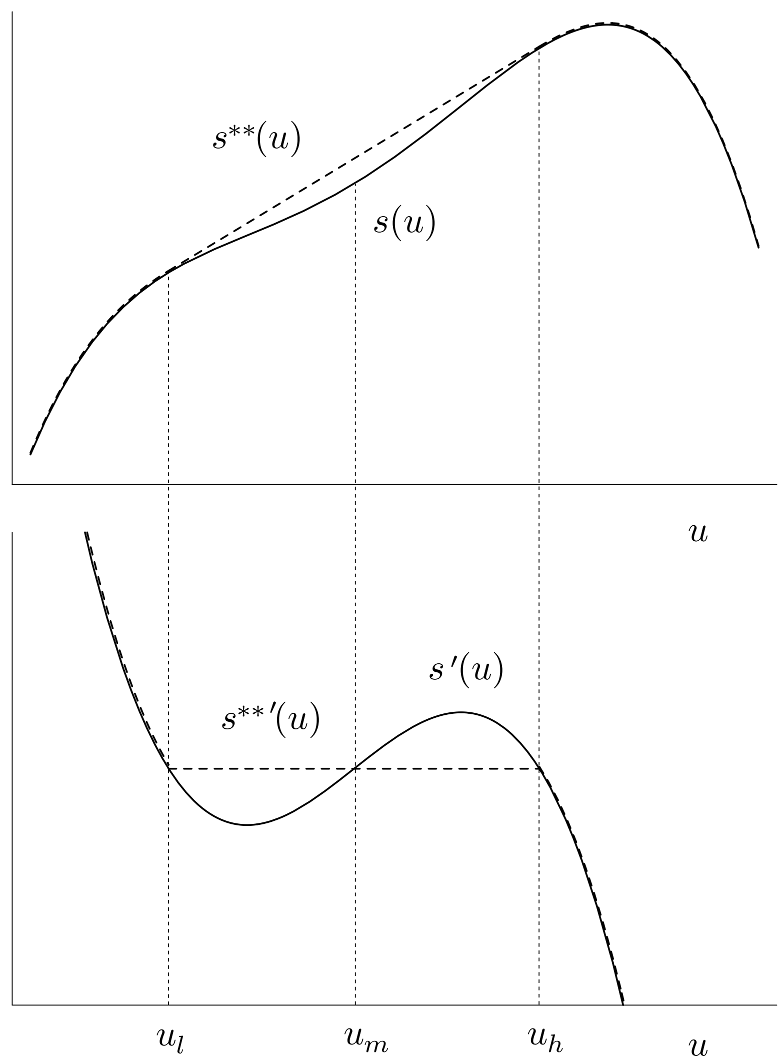
Macrostate equivalence $\Longleftrightarrow$ thermodynamic equivalence



Concave hull s^{**} of s

Define $s^{**} = (s^*)^*$, double-Legendre-Fenchel transform of s.
s^{**} equals the u.s.c. concave hull of s.

- Define s concave at u if $s(u) = s^{**}(u)$.
- Define s strictly concave at u if $s(u) = s^{**}(u)$ and s^{**} strictly concave at u.
- Define s nonconcave at u if $s(u) \neq s^{**}(u)$.



Rigorous results: microcanonical ensemble is more basic

RSE, Kyle Haven, Bruce Turkington (*JSP*, 2000)

$$\mathcal{E}^u \doteq \{\nu \in \mathcal{X} : I(\nu) \text{ is minimized for } f(\nu) = u\}$$

$$\mathcal{E}_\beta \doteq \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) \text{ is minimized}\}$$

- **Full equivalence of ensembles:**
  $s(u) \doteq -\inf\{I(\nu) : f(\nu) = u\}$ strictly concave at u
  $\Rightarrow \mathcal{E}^u = \mathcal{E}_\beta$ for unique β
  $\Rightarrow$ canonical $\equiv$ microcanonical

- **Nonequivalence of ensembles:**
  $s(u)$ nonconcave at u
  $\Rightarrow \mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β
  $\Rightarrow$ microcanonical not realized within canonical

- **Partial equivalence of ensembles:**
  $s(u)$ (not strictly) concave at $u \Rightarrow \mathcal{E}^u \subsetneq \mathcal{E}_\beta$ for unique β

- **Canonical ensemble is always realized within microcanonical ensemble:**

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

Generalizations and Applications

- Canonical equilibrium macrostates are always realized microcanonically. However, if s is not concave at u, then the microcanonical equilibrium macrostates are not realized canonically.

- Conclusion: the microcanonical ensemble is richer and more basic than the canonical ensemble.

- In classical models such as the Ising spin model, I is affine or convex and f is affine. Thus

$$s(u) = -\inf\{I(\nu) : \nu \in \mathcal{X}, f(\nu) = u\}$$

  is concave. Full or partial equivalence of ensembles holds.

- Models of turbulence show additional features.

  - All our results generalize to multidimensional cases in which s is a function of energy u, enstrophy, circulation, and other quantities conserved by the underlying p.d.e.

  - The most spectacular application of statistical theories of turbulence is to the prediction of large scale, coherent structures of the atmosphere of Jupiter including the Great Red Spot.

  - The microcanonical equilibrium macrostates not realized canonically often include macrostates of physical interest; e.g., the Great Red Spot of Jupiter.

■ Mean-field Blume-Emery-Griffiths (BEG) spin model

M. Blume, V. J. Emery, R. B. Griffiths (1971)

□ Definition of the model

- n spins $\omega_i \in \{-1, 0, +1\}$
- Microstates: $\omega \doteq (\omega_1, \omega_2, \ldots, \omega_n) \in \{-1, 0, 1\}^n$
- Hamiltonian:

$$\begin{aligned} H_n(\omega) &= \sum_{i=1}^n \omega_i^2 - \frac{K}{n} \left(\sum_{i=1}^n \omega_i\right)^2 \\ &= \underbrace{N_{n,1} + N_{n,-1}}_{\text{noninteracting}} - \frac{K}{n} \underbrace{\left(N_{n,1} - N_{n,-1}\right)^2}_{\text{magnetization}}, \end{aligned}$$

$$N_{n,j} \doteq \sum_{i=1}^n 1_j\{\omega_i\} = \#\{i : \omega_i = j\}$$

- Energy per particle:

$$h_n(\omega) \doteq \frac{1}{n} H_n(\omega) = L_{n,1} + L_{n,-1} - K(L_{n,1} - L_{n,-1})^2$$

- Macroscopic variable (empirical vector):

$$L_n = (L_{n,-1}, L_{n,0}, L_{n,1}),$$

$$L_{n,j}(\omega) \doteq \frac{1}{n} \sum_{i=1}^n 1_j(\omega_i) = \frac{1}{n} \cdot \#\{i : \omega_i = j\},$$

$$L_{n,j} \geq 0, L_{n,-1} + L_{n,0} + L_{n,1} = 1 \implies L_n(\omega) \in \mathcal{P}(\{-1, 0, 1\})$$

- A priori measure:

$$P_n(\omega) \doteq \frac{1}{3^n} \text{ for each } \omega$$

□ Large deviation analysis of the mean-field BEG model

- A priori measure:

$$P_n(\omega) \doteq \frac{1}{3^n} \text{ for each } \omega$$

- Energy per particle:

$$h_n(\omega) \doteq L_{n,1} + L_{n,-1} - K(L_{n,1} - L_{n,-1})^2$$

- Macroscopic variable (empirical vector):

$$L_n = (L_{n,-1}, L_{n,0}, L_{n,1}),$$
$$L_{n,j}(\omega) \doteq \frac{1}{n} \sum_{i=1}^n 1_j(\omega_i) = \frac{1}{n} \cdot \#\{i : \omega_i = j\}$$

  - Energy representation function:

    $$h_n(\omega) = f(L_n(\omega)),\ f(\nu) \doteq \nu_1 + \nu_{-1} - K(\nu_1 - \nu_{-1})^2$$

    for $\nu = (\nu_{-1}, \nu_0, \nu_1) \in \mathcal{P}(\{-1, 0, 1\})$

  - Basic LDP:

    $$P_n\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nR(\nu)}$$

    Sanov's Theorem gives rate function

    $$R(\nu) \doteq \nu_{-1} \log(3\nu_{-1}) + \nu_0 \log(3\nu_0) + \nu_1 \log(3\nu_1),$$

    relative entropy of $\sum_{j=-1}^1 \nu_j \delta_j$ w.r.t. $\sum_{j=-1}^1 \frac{1}{3}\delta_j$

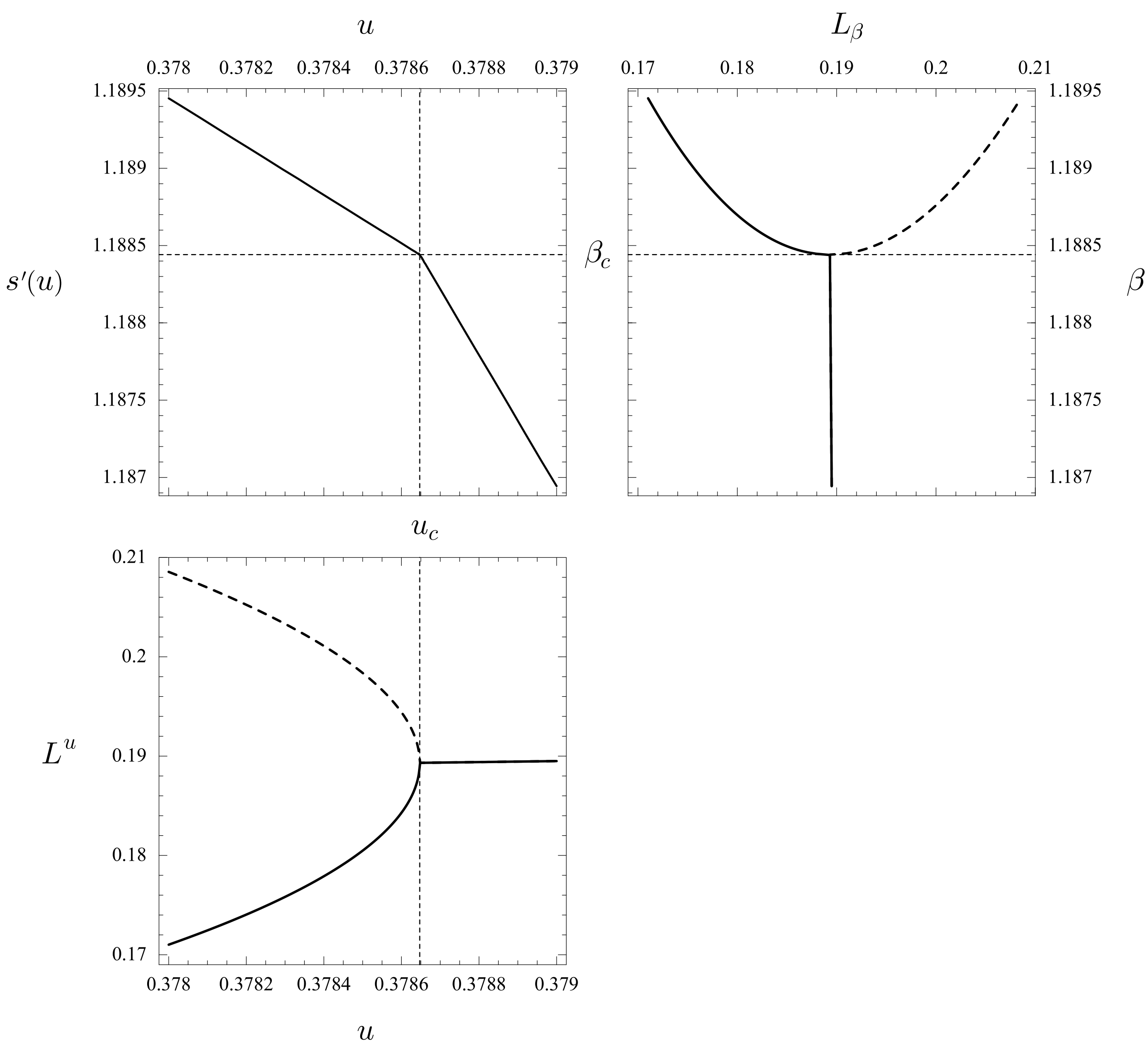
- Equilibrium macrostates:

$$L^u \doteq \arg\inf_\nu \{R(\nu) : f(\nu) = u\}$$
$$L_\beta \doteq \arg\inf_\nu \{R(\nu) + \beta f(\nu)\}$$

□ Exact comparison of equilibrium macrostates

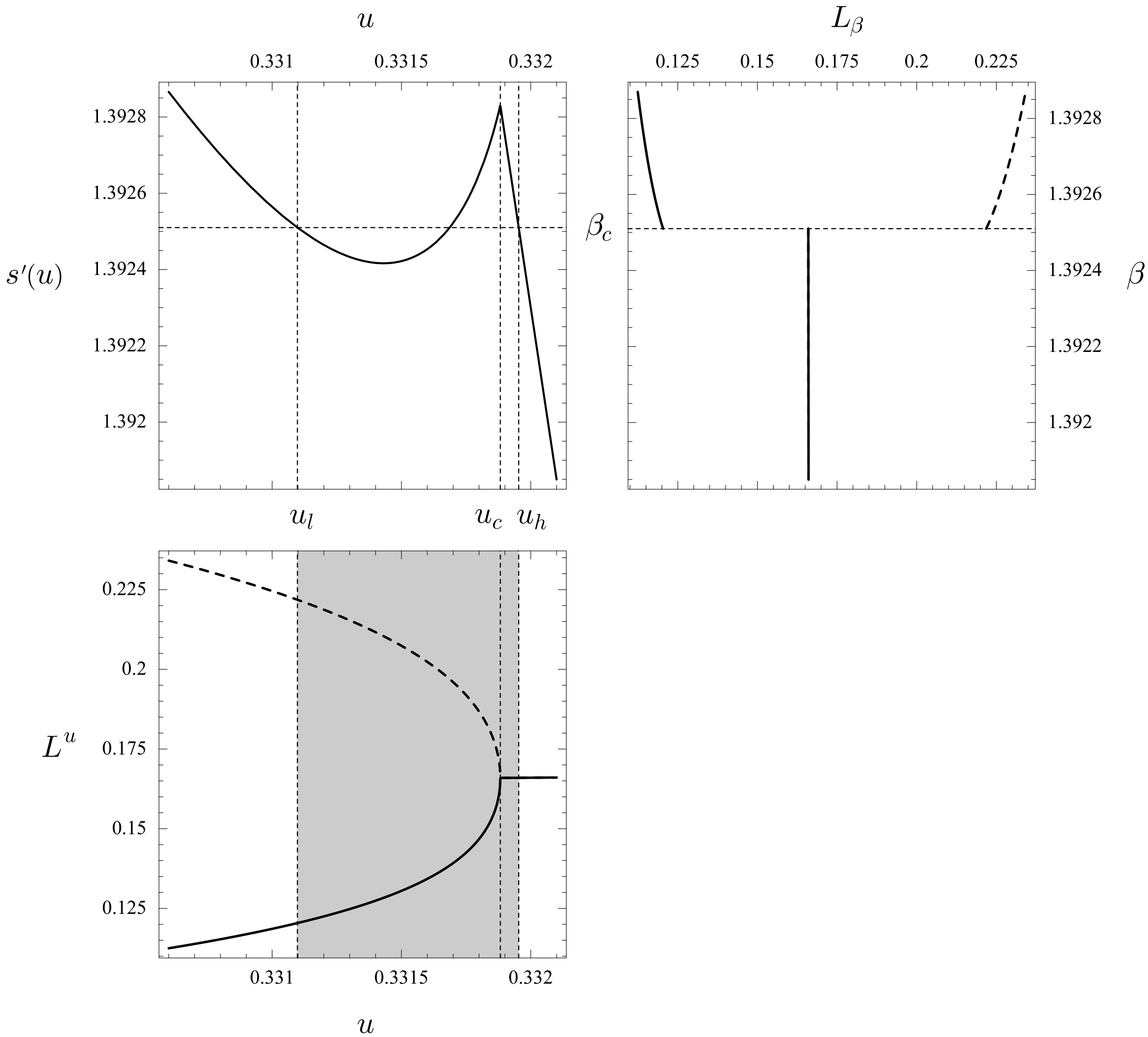
$$s(u) \doteq -\inf\{R(\nu) : \underbrace{\nu_1 + \nu_{-1} - K(\nu_1 - \nu_{-1})^2}_{f(\nu)\ \text{concave}} = u\}$$

$K = 1.111111111$



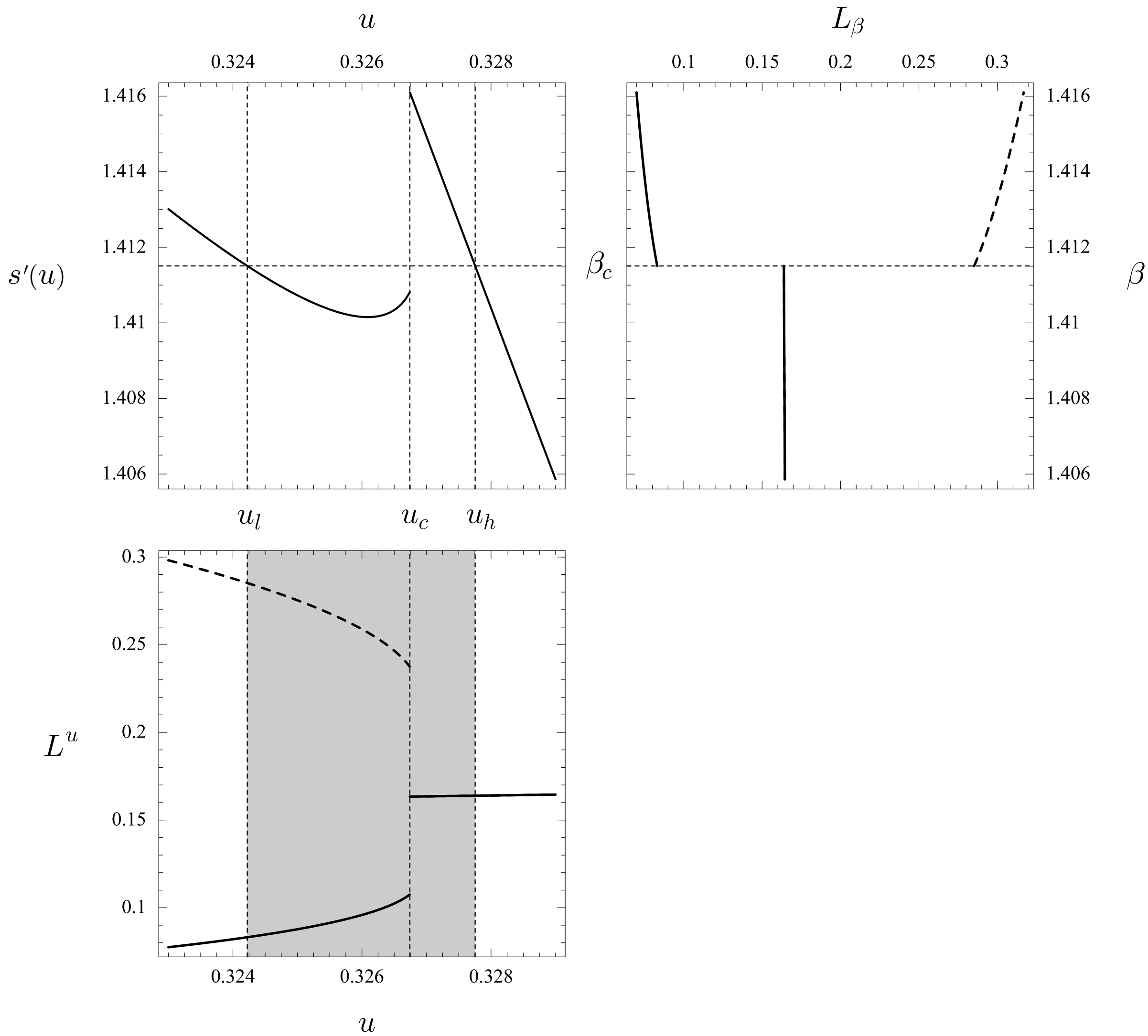
- s' monotonically decreasing $\Rightarrow$ s strictly concave
- Complete equivalence of ensembles
- Continuous phase transitions in β and u

$K = 1.081651726$



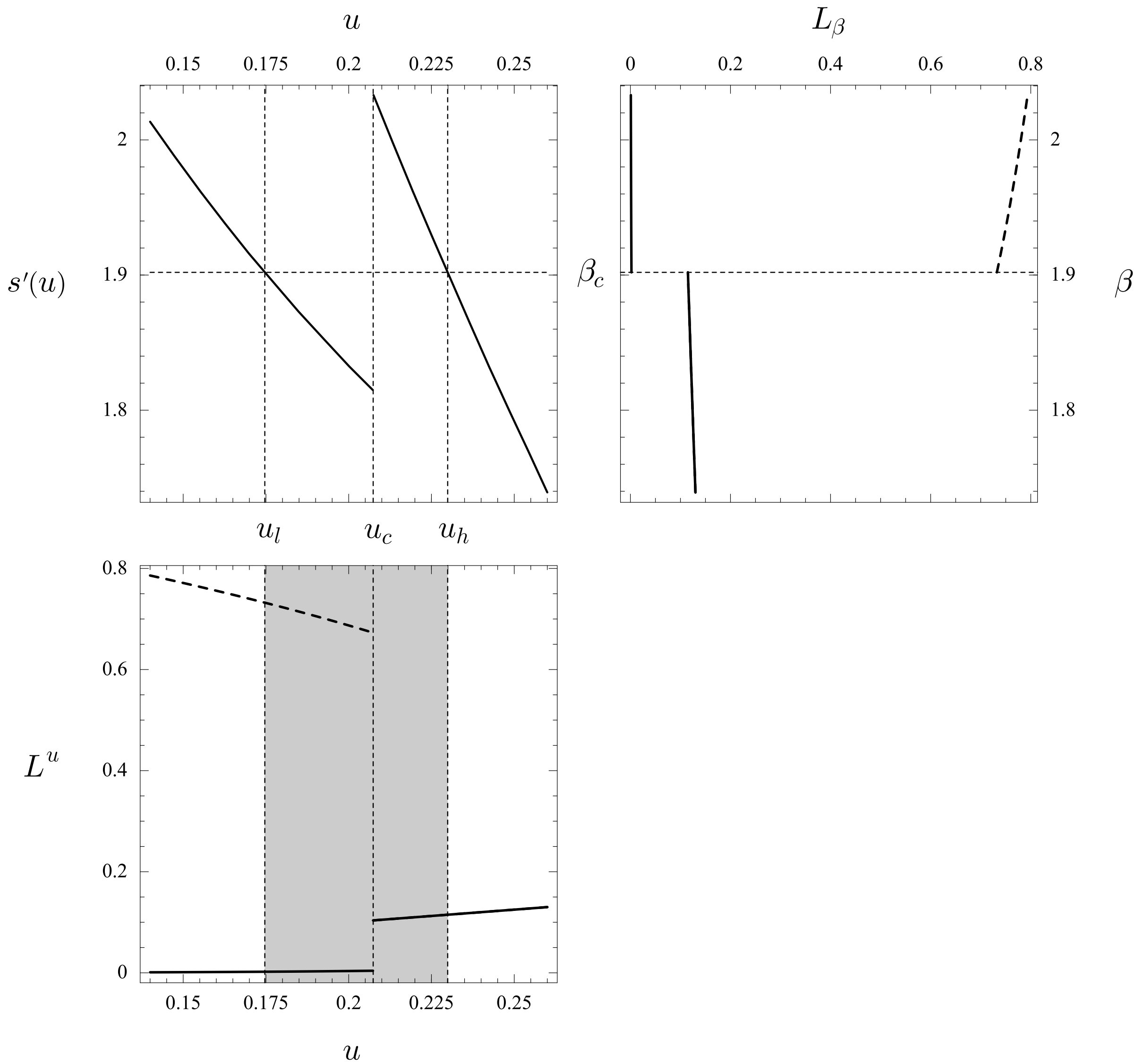
- s' not decreasing $\Rightarrow s$ not concave
- $s(u) \neq s^{**}(u)$ for $u_l \doteq 0.3311 < u < u_h \doteq 0.33195$
- Canonical ph. tr. at β_c defined by Maxwell-equal-area line
- Nonequivalence of ensembles: for $u_l < u < u_h$ L^u is not realized by L_β for any β: $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β.
- First-order phase transition in β versus second-order in u

$K = 1.080501698$



- s' not decreasing $\Rightarrow s$ not concave
- $s(u) \neq s^{**}(u)$ for $u_l \doteq 0.32425 < u < u_h \doteq 0.32775$
- Canonical ph. tr. at β_c given by Maxwell-equal-area line
- Nonequivalence of ensembles: for $u_l < u < u_h$ L^u is not realized by L_β for any β: $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β.
- First-order phase transitions in β and u

$K = 1.050001050$



- Similar features as on preceding transparency: nonequivalence of ensembles and first-order phase transitions in β and u

Conclusion

- Convexity theory and large deviation theory provide powerful methodology for studying equivalence and nonequivalence of ensembles.

- BEG model illustrates macrostate nonequivalence of ensembles: canonical $\neq$ microcanonical.

- Microcanonical ensemble is **richer** than canonical ensemble.

- In models of turbulence, the microcanonical equilibrium macrostates not realized as canonical equilibrium macrostates include macrostates of physical interest.

- Canonical ensemble is **always realized** within microcanonical ensemble.

- Macrostate nonequivalence of ensembles is associated with **nonconcavity** of $s(u)$.

- Macrostate nonequivalence of ensembles is associated with **nondifferentiability** of $\varphi(\beta)$ (canonical first-order phase transition).

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□ BEG Model

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