Global Optimization, the Gaussian Ensemble, and Universal Ensemble Equivalence

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June 2005

Research supported by a grant from the National Science Foundation (NSF-DMS-0202309)
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■ Outline of the Talk

- Physical motivation
  - Equivalence of microcanonical, canonical, and Gaussian ensembles
  - Analyze equivalence at the level of equilibrium macrostates
  - Microcanonical equilibrium macrostates need not be canonical equilibrium macrostates, but in general are Gaussian equil. macrostates.
  - Great Red Spot of Jupiter and stability analysis
- Three related minimization problems
  - Constrained minimization: microcanonical ensemble
  - Unconstrained minimization with a Lagrange multiplier: canonical ensemble
  - Unconstrained minimization with a Lagrange multiplier and a penalty function: Gaussian ensemble
- Relationships among the solutions of the three problems
  - Determined by concavity properties of the microcanonical entropy and the generalized microcanonical entropy
  - From nonequivalence to universal equivalence
- Statistical mechanical ensembles
  - Large deviation methodology
- Two theorems on ensemble equivalence and nonequivalence
- Results for Curie-Weiss-Potts model
- References
  - Ensemble equivalence: *J. Stat. Phys.* (2000)
  - Universal ensemble equivalence: *J. Stat. Phys.* (2005)
  - Stability analysis: *Nonlinearity* (2002)
  - Curie-Weiss-Potts model: *J. Math. Phys.* (2005) and in preparation

Physical Motivation

Define Gaussian ensemble via measure

$$P_{n,\beta,\gamma}(\omega) = \text{const} \cdot P_{n,\beta}(\omega)\, e^{-n\gamma[h_n(\omega)]^2},$$

$$P_{n,\beta} = \text{ measure defining canonical ensemble}$$

$$h_n = \text{ energy per particle}$$

For energy u, inverse temperature β, and penalty parameter γ

- $\mathcal{E}^u$ = set of microcanonical equilibrium macrostates
- $\mathcal{E}_\beta$ = set of canonical equilibrium macrostates
- $\mathcal{E}(\gamma)_\beta$ = set of Gaussian equilibrium macrostates

Basic problem. What are the relationships among these 3 sets?

- For fixed β, $\mathcal{E}_\beta \subset \mathcal{E}^u$ for some u
- For fixed u
  - ◦ $\mathcal{E}^u \subset \mathcal{E}_\beta$ for some β (equivalence)
  - ◦ $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β (nonequivalence)
- If $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β, can we recover equivalence via the Gaussian ensemble?
  - ◦ Want β and γ such that $\mathcal{E}^u \subset \mathcal{E}(\gamma)_\beta$

Analyze equivalence and nonequivalence via concavity properties of two functions

- Microcanonical entropy $s(u)$
- Generalized microcanonical entropy $s(u) - \gamma u^2$

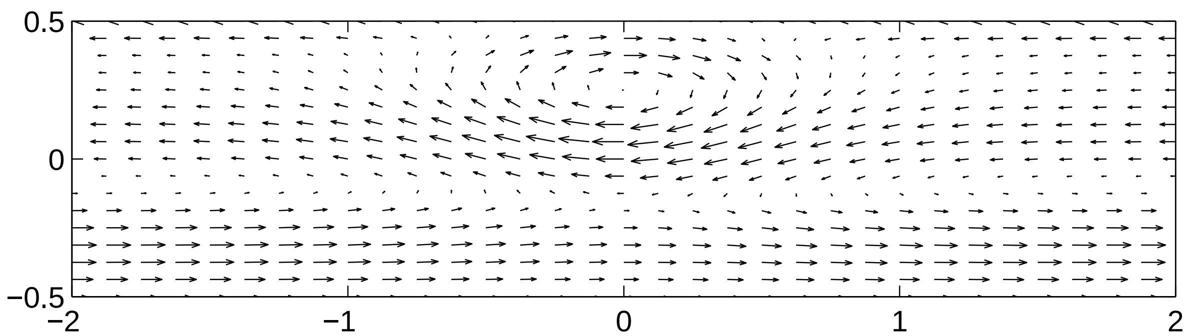
Statistical Theories of Turbulence

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

- Apply statistical theories of turbulence to predict 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. Prove their stability via an analysis based on the Gaussian ensemble.

Using a simplified model in *Nonlinearity* (2002) based on a sinusoidal topography, we generate a coherent anticyclonic vortex within a zonal shear having multiple flow reversals and resembling the Great Red Spot of Jupiter.



- This flow is in $\mathcal{E}^u$ but not in $\mathcal{E}_\beta$ for any β.
- Its stability cannot be proved via the standard Arnold stability theorems.
- We prove stability using a Lyapunov function based on the Gaussian ensemble.
- This flow is either a Gaussian metastable macrostate (local minimum of rate function) or a Gaussian equilibrium macrostate (global minimum of rate function).

Three Related Minimization Problems

- $\mathcal{X}$ a space
- I a nonnegative function on $\mathcal{X}$
- f a real-valued function on $\mathcal{X}$

Investigate the relationships among solutions of three minimization problems.

1. Constrained minimization for given u:

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

2. Unconstrained minimization for given β:

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

   β a Lagrange multiplier

3. Unconstrained minimization for given β, γ, u:

   $\mathcal{E}(\gamma)^u_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma[f(\nu) - u]^2 \text{ is minimized}\}$

   $\gamma[f(\nu) - u]^2$ a penalty function

Rewrite $\mathcal{E}(\gamma)_\beta^u$

$$\mathcal{E}(\gamma)_\beta^u = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma[f(\nu) - u]^2 \text{ is minimized}\}$$

- As $\gamma \to \infty$, $\gamma[f(\nu) - u]^2 \to \delta_u(f(\nu))$.
- This gives constraint in

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

- Work with large $\gamma > 0$.

$$\mathcal{E}(\gamma)_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma[f(\nu)]^2 \text{ is minimized}\}$$

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

$$\mathcal{E}_\beta = \mathcal{E}(0)_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) \text{ is minimized}\}$$

$\mathcal{E}^u$, $\mathcal{E}_\beta$, and $\mathcal{E}(\gamma)_\beta$ express the asymptotic behavior of the microcanonical ensemble, the canonical ensemble, and the Gaussian ensemble. Derive via large deviations.

Theorem (RSE, KH, BT)

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

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

$$\mathcal{E}(\gamma)_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma[f(\nu)]^2 \text{ is minimized}\}$$

Only 4 relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$.

Theorem (*JSP*, 2000)

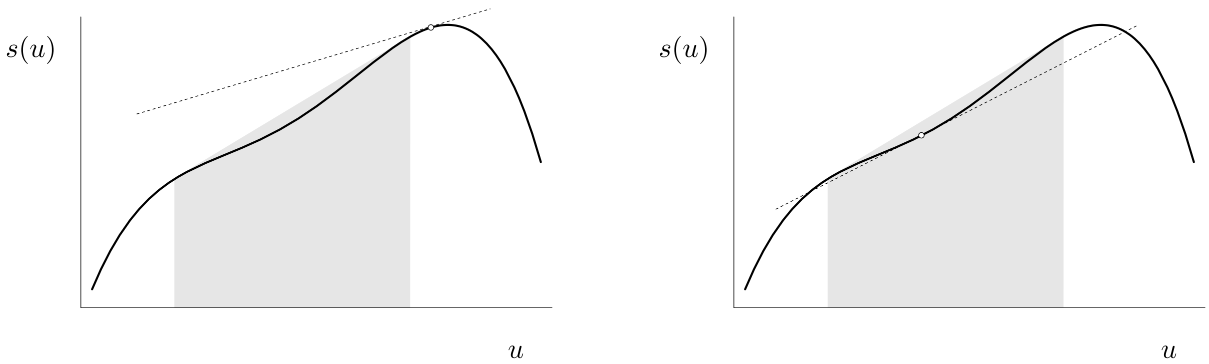
1. Fix β. Then $\exists u$ such that $\nu \in \mathcal{E}_\beta \Rightarrow \nu \in \mathcal{E}^u$.
2. Fix u. Can we always find β such that $\nu \in \mathcal{E}^u \Rightarrow \nu \in \mathcal{E}_\beta$?
   (a) **Full equivalence.** $\exists \beta$ such that $\mathcal{E}^u = \mathcal{E}_\beta$.
   (b) **Partial equivalence.** $\exists \beta$ such that $\mathcal{E}^u \subset \mathcal{E}_\beta$ but $\mathcal{E}^u \neq \mathcal{E}_\beta$.
   (c) **Nonequivalence.** $\forall \beta \;\; \mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$.

- Give criteria for 2(a), 2(b), and 2(c) in terms of concavity properties of the microcanonical entropy

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

  - s strictly concave at (all) $u \Rightarrow$ full equivalence for (all) u
  - s (not strictly) concave at $u \Rightarrow$ partial equivalence for u
  - s not concave on subset $A \Rightarrow$ nonequivalence $\forall u \in A$.
- Is there a similar theorem relating $\mathcal{E}^u$ and $\mathcal{E}(\gamma)_\beta$? Give criteria for full equivalence, partial equivalence, and nonequivalence in terms of concavity properties of what function?

Example of Microcanonical Entropy



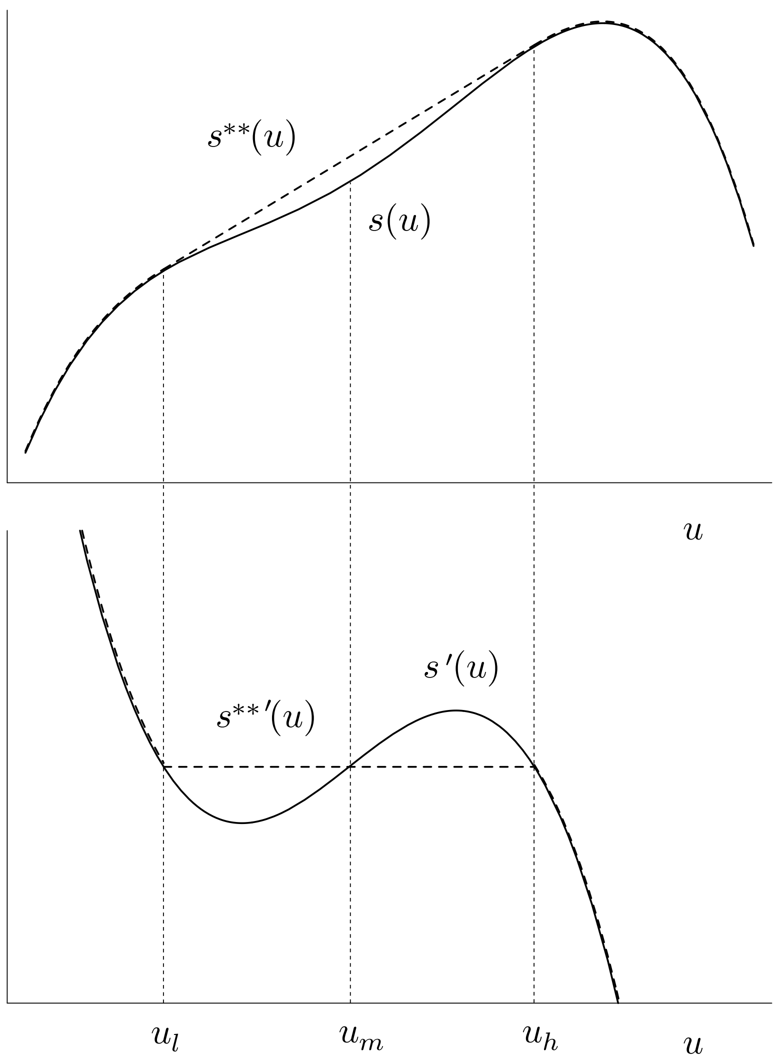
Denote by u_ℓ and u_h the projection of the shaded region onto the u axis.

- For $u < u_\ell$ and $u > u_h$, s is strictly concave (strictly supporting line), and we have full equivalence.
- For $u = u_\ell$ and $u = u_h$, s is concave but not strictly concave (nonstrictly supporting line), and we have partial equivalence.
- For $u_\ell < u < u_h$, s is not concave (no supporting line), and we have nonequivalence.

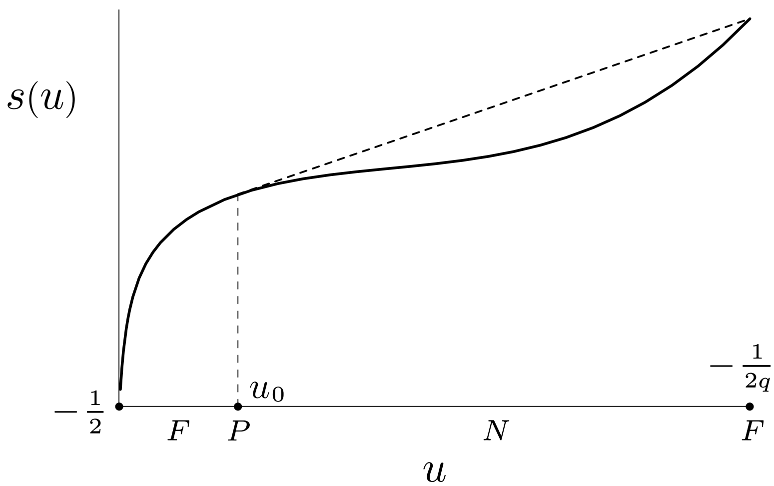
□ Concave hull s^{**} of s

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



□ $s(u)$ for the Curie-Weiss-Potts Model



For CWP model

$$\text{dom } s = \{u \in \mathbb{R} : s(u) < \infty\} = [-\tfrac{1}{2}, -\tfrac{1}{2q}].$$

Define

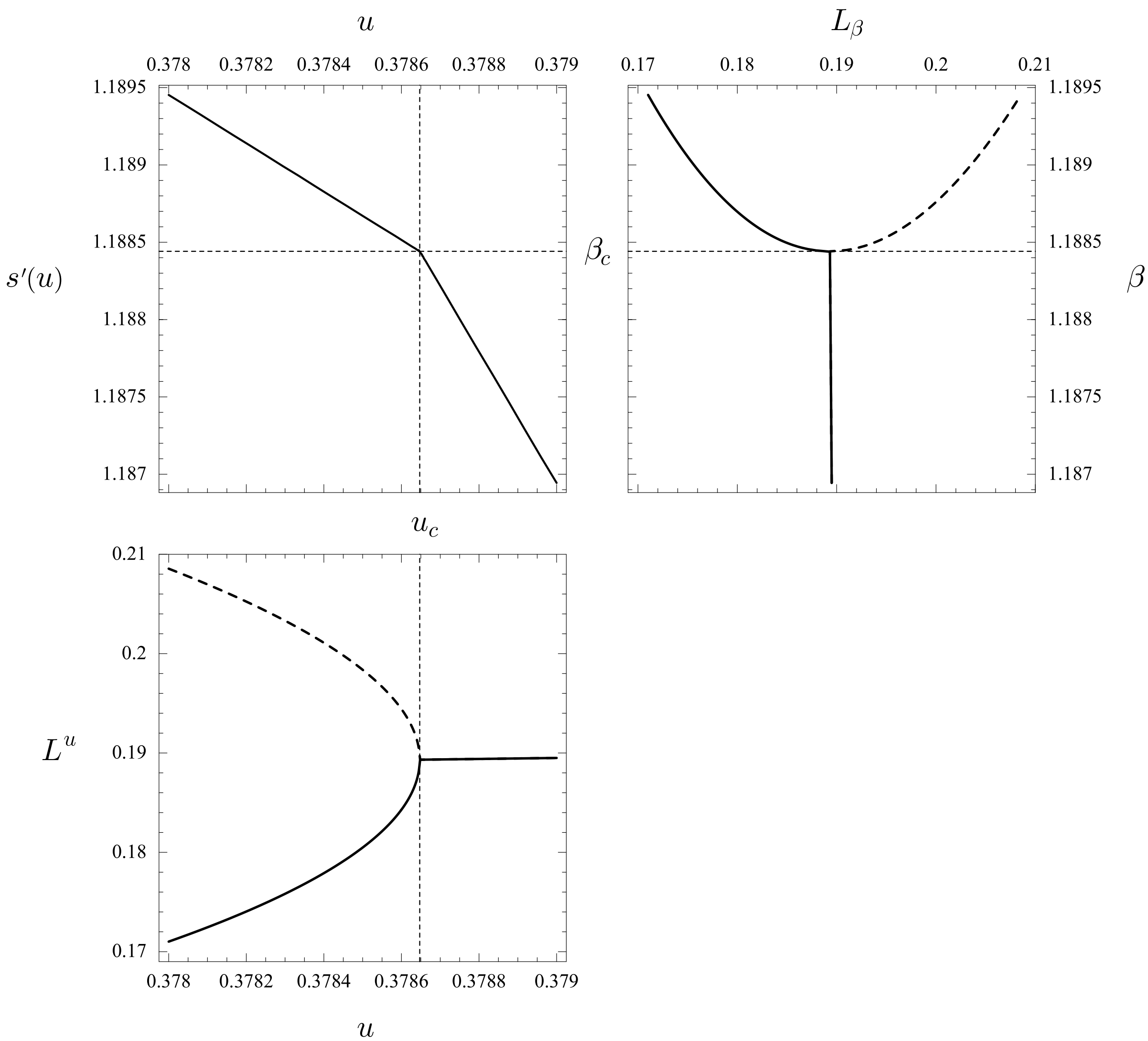
$$\begin{aligned} F &= \{u \in \text{dom } s : \mathcal{E}^u = \mathcal{E}_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ strictly concave at } u\}, \\ P &= \{u \in \text{dom } s : \mathcal{E}^u \subset \mathcal{E}_\beta \text{ but } \mathcal{E}^u \neq \mathcal{E}_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ (not strictly) concave at } u\}, \\ N &= \{u \in \text{dom } s : \mathcal{E}^u \neq \mathcal{E}_\beta \text{ for any } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ not concave at } u\}. \end{aligned}$$

Theorem (*JMP*, 2005). There exists $u_0 \in (-\frac{1}{2}, -\frac{1}{2q})$ such that

$$\begin{aligned} F &= (-\tfrac{1}{2}, u_0) \cup \{-\tfrac{1}{2q}\}, \\ P &= \{u_0\}, \\ N &= (u_0, -\tfrac{1}{2q}). \end{aligned}$$

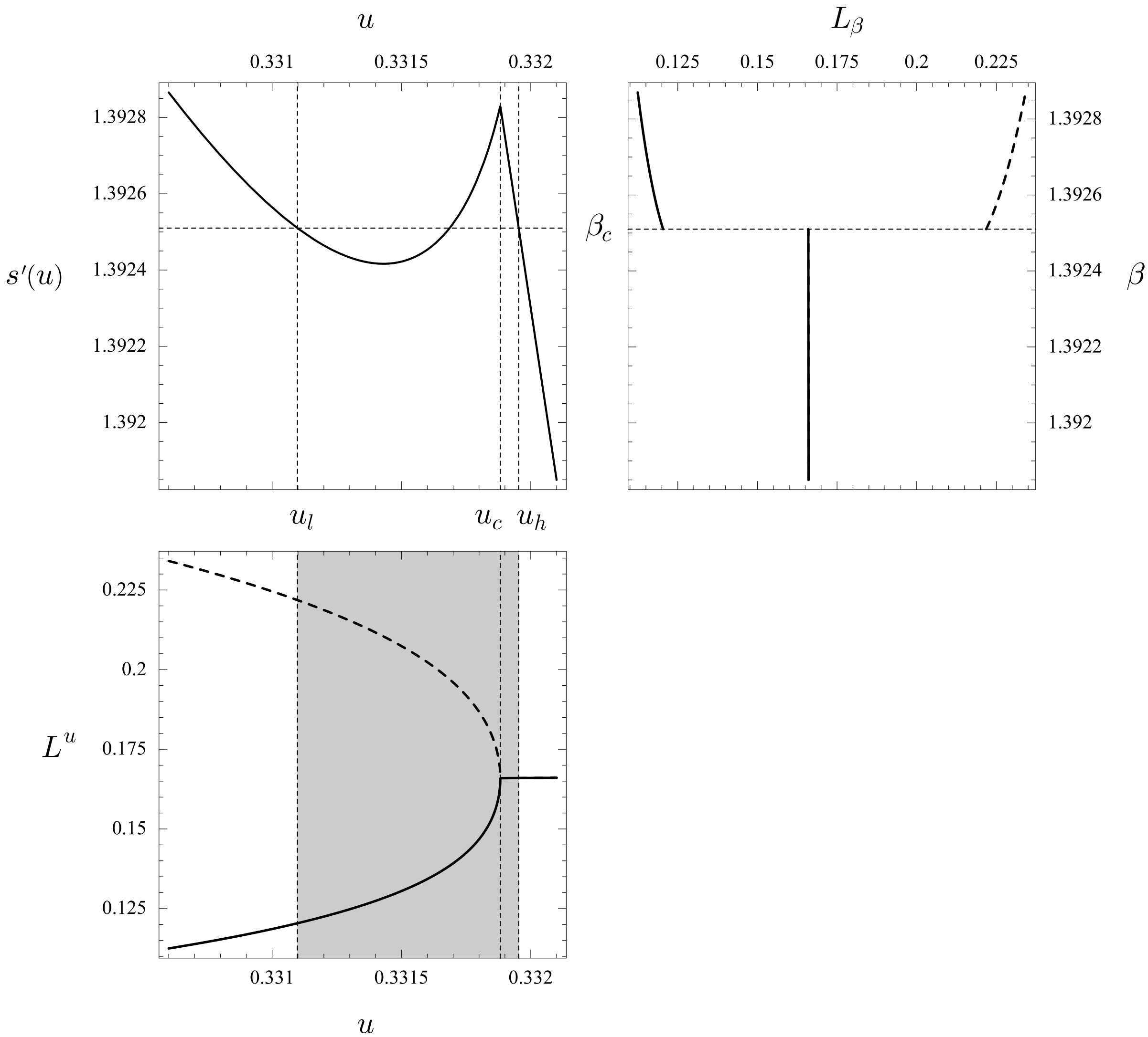
□ $\mathcal{E}_\beta$, $s'(u)$, and $\mathcal{E}^u$ for the BEG Model

$K = 1.111111111$ in the mean-field Blume-Emery-Griffiths (BEG) model



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

$K = 1.081651726$ in the mean-field BEG model



- s' not decreasing $\Rightarrow s$ not concave
- $s(u)$ not concave for $u_l = 0.3311 < u < u_h = 0.33195$
- 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

From Nonequivalence to Universal Equivalence (MC, RSE, HT, BT)

$$\mathcal{E}^u = \{\nu \in \mathcal{X} : I(\nu) \text{ is minimized for } f(\nu) = u\}$$
$$\mathcal{E}_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) \text{ is minimized}\}$$
$$\mathcal{E}(\gamma)_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma[f(\nu)]^2 \text{ is minimized}\}$$

Problem. Suppose that for all β and a subset A of u

$$\text{nonequivalence: } \mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset.$$

Find $\gamma > 0$ and β such that for all u

$$\text{universal equivalence: } \mathcal{E}^u = \mathcal{E}(\gamma)_\beta.$$

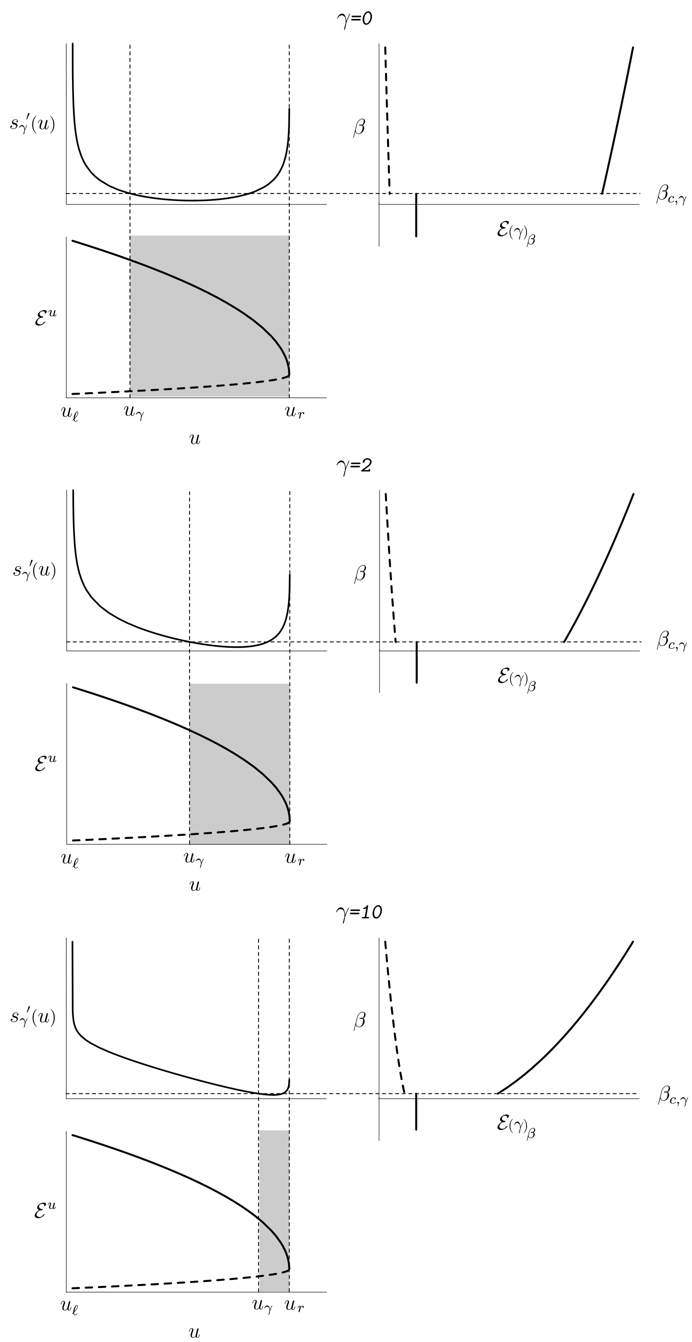
Surprise. The simplicity with which γu^2 enters the formulation.

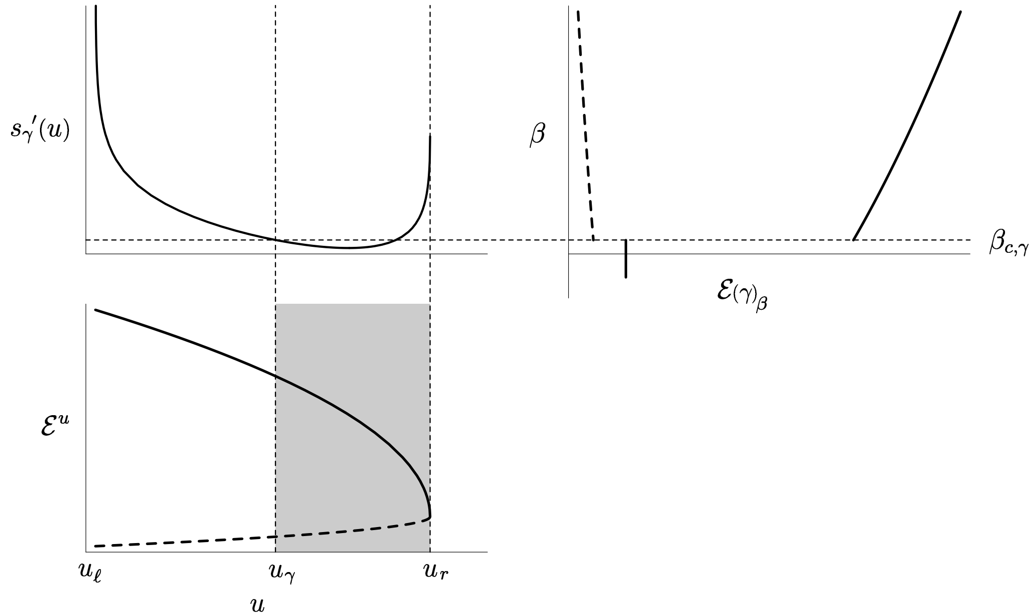
Theorem. Define $s(u) = -\inf\{I(\nu) : \nu \in \mathcal{X}, f(\nu) = u\}$.

1. $s(u)$ strictly concave $\Rightarrow \exists\beta$ such that $\mathcal{E}^u = \mathcal{E}_\beta$.
2. $s(u) - \gamma u^2$ strictly concave $\Rightarrow \exists\beta$ such that $\mathcal{E}^u = \mathcal{E}(\gamma)_\beta$.
3. Assume: s is C^2, not strictly concave, and s'' is bounded above. Choose $\gamma > \frac{1}{2}s''(u)$ for all u. Then $s(u) - \gamma u^2$ is strictly concave for all u and $\exists\beta$ such that
$$\mathcal{E}^u = \mathcal{E}(\gamma)_\beta.$$
4. Assume: s is C^2, not strictly concave, and s'' is not bounded above. Then for each u $\exists\gamma_0 \geq 0$ and $\exists\beta$ such that $\forall\gamma > \gamma_0$
$$\mathcal{E}^u = \mathcal{E}(\gamma)_\beta.$$
As $\gamma \uparrow$, $\mathcal{E}(\gamma)_\beta$ picks up more $\nu \in \mathcal{E}^u$.

□ $\mathcal{E}(\gamma)_\beta$, $(s(u) - \gamma u^2)'$, and $\mathcal{E}^u$ for the CWP Model

- $\mathcal{E}(\gamma)_\beta$ for $\gamma = 0, 2, 10$; $(s(u) - \gamma u^2)'$; and $\mathcal{E}^u$
- Full equivalence left of vertical line in $(s(u) - \gamma u^2)'$ figure; as $\gamma \uparrow$, full equivalence region increases to $(u_\ell, u_r]$.





$$\text{dom } s = \{u \in \mathbb{R} : s(u) < \infty\} = [u_\ell, u_r] = [-\tfrac{1}{2}, -\tfrac{1}{2q}].$$

For $\gamma \geq 0$ define $s_\gamma(u) = s(u) - \gamma u^2$ and

$$\begin{aligned} F_\gamma &= \{u \in \text{dom } s : \mathcal{E}^u = \mathcal{E}(\gamma)_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s_\gamma \text{ strictly concave at } u\}, \\ P_\gamma &= \{u \in \text{dom } s : \mathcal{E}^u \subset \mathcal{E}(\gamma)_\beta \text{ but } \mathcal{E}^u \neq \mathcal{E}(\gamma)_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s_\gamma \text{ (not strictly) concave at } u\}, \\ N_\gamma &= \{u \in \text{dom } s : \mathcal{E}^u \neq \mathcal{E}(\gamma)_\beta \text{ for any } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s_\gamma \text{ not concave at } u\}. \end{aligned}$$

Theorem. There exists $u_\gamma \in (u_\ell, u_r) = (-\frac{1}{2}, -\frac{1}{2q})$ such that

$$F_\gamma = (u_\ell, u_\gamma) \cup \{u_r\},\ P_\gamma = \{u_\gamma\},\ N_\gamma = (u_\gamma, u_r).$$

As $\gamma \to \infty$, $u_\gamma \uparrow u_r$, $F_\gamma \uparrow (u_\ell, u_r]$, and $\beta_{c,\gamma} \to \infty$, where $\beta_{c,\gamma} = s'_\gamma(u_\gamma)$ is the value of β at which $\mathcal{E}(\gamma)_\beta$ has a first-order phase transition.

Physical Background

Two classical choices of probability distributions in equilibrium statistical mechanics:

$$\boxed{\begin{array}{c}\textbf{Microcanonical}\text{ ensemble}\\ u = \text{const}\end{array}}$$

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

$$\boxed{\begin{array}{c}\textbf{Canonical}\text{ ensemble}\\ \beta \text{ or } T = \text{const}\end{array}}$$

Also Gaussian ensemble = canonical ensemble with a penalty function

- Are the probability distributions equivalent?
- Can microcanonical equilibrium macrostates always be realized canonically?
  - Classical answer: yes.
  - Modern theory: in general no.
- Can microcanonical equilibrium macrostates always be realized in the Gaussian ensemble? In general yes.
- Equivalence of ensembles:
  - Example: perfect gas
  - General conditions: short-range interactions

Examples of Systems Having Nonequivalent Ensembles

- Gravitational systems: Lynden-Bell (1968), Thirring (1970), Gross (1997, 2001)
- Lennard-Jones gas: Borges and Tsallis (2002)
- Plasma models: Smith and O'Neil (1990)
- Spin models
  - Curie-Weiss-Potts model: Costeniuc, Ellis, and Touchette (2004)
  - Half-blocked spin model: Touchette (2003)
  - Hamiltonian mean-field model: Latora, Rapisarda, and Tsallis (2001)
  - Mean-field Blume-Emery-Griffiths model
    - Thermo level: Barré, Mukamel, and Ruffo (2002)
    - Macro level: Ellis, Touchette, and Turkington (2004)
  - Mean-field XY model: Dauxois, Holdsworth, and Ruffo (2000)
- Turbulence models: Robert and Sommeria (1991); Caglioti, Lions, Marchioro, and Pulvirenti (1992); Kiessling and Lebowitz (1997); Ellis, Haven, and Turkington (2002)

Statistical Mechanical Ensembles

Boltzmann (1872), Gibbs (1876, 1902)

1. ω_i, $i = 1, 2, \ldots, n$, each $\omega_i \in \Lambda$ (spins or vorticities or $\ldots$)

2. Microstates: $\omega = (\omega_1, \omega_2, \ldots, \omega_n) \in \Lambda^n$

3. Hamiltonian or energy function: $H_n(\omega)$

4. Energy per particle: $h_n(\omega) = \frac{1}{n} H_n(\omega)$

5. Prior measure P_n; e.g., if Λ is a finite set,

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

6. 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 $\ldots$).

   (a) $\mathcal{X}$ is space of macrostates.

   (b) Require bounded, continuous energy representation function f mapping $\mathcal{X}$ into $\mathbb{R}$: as $n \to \infty$

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

   (c) 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-Potts (CWP) Spin Model

Approximation to the Potts model (Wu (1982))

1. n spins $\omega_i \in \Lambda = \{1, 2, \ldots, q\}$, $q \geq 3$
2. Microstates: $\omega = (\omega_1, \omega_2, \ldots, \omega_n) \in \Lambda^n$
3. Hamiltonian or energy function:
$$H_n(\omega) = -\frac{1}{2n} \sum_{j,k=1}^n \delta(\omega_j, \omega_k)$$
4. Energy per particle:
$$h_n(\omega) = \frac{1}{n} H_n(\omega)$$
5. Prior measure:
$$P_n(\omega) = \frac{1}{q^n} \text{ for each } \omega \in \Lambda^n$$
6. Macroscopic variable (empirical vector):
$$L_n = (L_{n,1}, L_{n,2}, \ldots, L_{n,q}),$$
$$L_{n,i}(\omega) = \frac{1}{n} \sum_{j=1}^n 1_i(\omega_j) = \frac{1}{n} \cdot \#\{j : \omega_j = i\},$$
$$L_{n,i} \geq 0, \sum_{i=1}^q L_{n,i} = 1 \implies L_n(\omega) \in \mathcal{P}(\mathbb{R}^q)$$
   (a) $\mathcal{P}(\mathbb{R}^q)$ is space of macrostates.
   (b) Energy representation function:
$$h_n(\omega) = -\frac{1}{2}\langle L_n(\omega), L_n(\omega)\rangle = f(L_n(\omega)),$$
$$f(\nu) = -\frac{1}{2}\langle \nu, \nu\rangle \text{ for } \nu \in \mathcal{P}(\mathbb{R}^q)$$
   (c) Basic LDP:
$$P_n\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nR(\nu)}$$
   Sanov's Theorem gives rate function
$$R(\nu) = \sum_{i=1}^q \nu_i \log(q\nu_i),$$
   relative entropy of $\sum_{i=1}^q \nu_i \delta_i$ with respect to $\sum_{i=1}^q \frac{1}{q}\delta_i$

□ Models to which the formalism has been applied

- Miller-Robert model of fluid turbulence based on the 2D Euler equations (CB, RSE, BT)

- Model of geophysical flows based on equations describing barotropic, quasi-geostrophic turbulence (RSE, KH, BT)

- Model of soliton turbulence based on a class of generalized nonlinear Schrödinger equations (RSE, RJ, PO, BT)

- Mean-field Blume-Emery-Griffiths spin model (RSE, PO, HT, BT)

- Curie-Weiss-Potts spin model (MC, RSE, HT)
  - $\mathcal{E}^u$ and $\mathcal{E}_\beta$ known explicitly
  - Detailed information concerning ensemble equivalence and nonequivalence
    - Nonequivalence. $\exists u$ such that $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β.
    - Equivalence via Gaussian ensemble. For all such u $\exists \gamma$ such that for all $v \leq u$

$$\mathcal{E}^v = \mathcal{E}(\gamma)_\beta \text{ for some } \beta = \beta(\gamma, v).$$

- Prior measure: $P_n(\{\omega\}) = \frac{1}{|\Lambda|^n}$ for each $\omega \in \Lambda^n$
- Assumption: $L_n(\omega)$ maps Λ^n into $\mathcal{X}$ such that
  - $h_n(\omega) = f(L_n(\omega)) + \mathrm{o}(1)$ 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

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

- 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 $s(u)$:

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

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

- 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 $L_n(\omega)$:

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

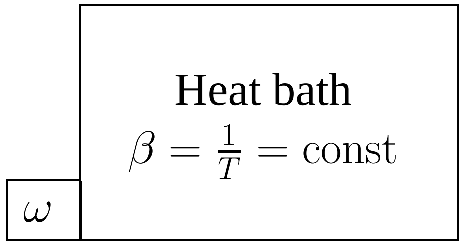
- Microcanonical equilibrium macrostates defined by $I^u(\nu) = 0$:

$I^u(\nu) \geq 0$ 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:

$$P_{n,\beta}(d\omega) = \frac{1}{Z_n(\beta)}\, e^{-\beta n h_n(\omega)}\, P_n(d\omega),$$

$$Z_n(\beta) = \int_{\Lambda^n} e^{-\beta n h_n}\, dP_n \asymp e^{-n\varphi(\beta)}$$

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

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

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

- 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 $I^u(\nu) = 0$:

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

□ Gaussian Ensemble $P_{n,\beta,\gamma}$

- Challa and Hetherington (1988), Johal et. al. (2003), Kiessling and Lebowitz (1997)

- Generalized Gibbs probability distribution (Gaussian ensemble):

$$P_{n,\beta,\gamma}(d\omega) = \frac{1}{Z_n(\beta,\gamma)} e^{-n\beta h_n(\omega) - n\gamma[h_n(\omega)]^2} P_n(d\omega),$$

$$Z_n(\beta,\gamma) = \int_{\Lambda^n} e^{-n\beta h_n - n\gamma[h_n]^2} dP_n \asymp e^{-n\varphi(\beta,\gamma)}$$

  $\varphi(\beta,\gamma)$ is the Gaussian free energy per particle.

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

$$\boxed{\begin{array}{c} P_{n,\beta,\gamma}\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI_{\beta,\gamma}(\nu)} \\ I_{\beta,\gamma}(\nu) = I(\nu) + \beta f(\nu) + \gamma[f(\nu)]^2 - \varphi(\beta,\gamma) \end{array}}$$

- Gaussian equilibrium macrostates defined by $I_{\beta,\gamma}(\nu) = 0$:
  $I_{\beta,\gamma}(\nu) \geq 0$ for all ν
  $I_{\beta,\gamma}(\nu) > 0 \Rightarrow P_{n,\beta,\gamma}\{\omega : L_n(\omega) \approx \nu\} \to 0$ exponentially fast

$$\boxed{\mathcal{E}(\gamma)_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma[f(\nu)]^2 \text{ is minimized}\}}$$

- Canonical equilibrium macrostates $\mathcal{E}_\beta = \mathcal{E}(0)_\beta$

- Microcanonical equilibrium macrostates:

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

Theorem 1: Microcanonical Ensemble More Basic Than Canonical Ensemble

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

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

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

- **Canonical is always realized microcanonically:**

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

- **Full equivalence of ensembles:**

  $s(u) = -\inf\{I(\nu) : f(\nu) = u\}$ strictly concave at u

  $\Rightarrow \mathcal{E}^u = \mathcal{E}_\beta$ for unique β

  $\Rightarrow$ canonical $\equiv$ microcanonical

- **Partial equivalence of ensembles:**

  s (not strictly) concave at $u \Rightarrow \mathcal{E}^u \subset \mathcal{E}_\beta$ for unique β but $\mathcal{E}^u \neq \mathcal{E}_\beta$

- **Nonequivalence of ensembles:**

  s not concave at u

  $\Rightarrow \mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all β

  $\Rightarrow$ microcanonical not realized canonically

Theorem 2: Universal Equivalence of Ensembles Is Possible

Marius Costeniuc, RSE, Hugo Touchette, Bruce Turkington (2004)

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

$$\mathcal{E}(\gamma)_\beta = \{\nu \in \mathcal{X} : I(\nu) + \beta f(\nu) + \gamma [f(\nu)]^2 \text{ is minimized}\}$$

- **Gaussian always realized microcanonically:**

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

- **Full equivalence of ensembles:**
  $s(u) - \gamma u^2$ strictly concave at u
  $\Rightarrow \mathcal{E}^u = \mathcal{E}(\gamma)_\beta$ for unique β
  $\Rightarrow$ Gaussian $\equiv$ microcanonical
  - **Universal equivalence of ensembles**: choose γ so that $s(u) - \gamma u^2$ is strictly concave for all u

- **Partial equivalence of ensembles:**
  $s(u) - \gamma u^2$ not strictly concave at $u \ \Rightarrow\ \mathcal{E}^u \subset \mathcal{E}(\gamma)_\beta$ for unique β but $\mathcal{E}^u \neq \mathcal{E}(\gamma)_\beta$

- **Nonequivalence of ensembles:**
  $s(u) - \gamma u^2$ not concave at u
  $\Rightarrow \mathcal{E}^u \cap \mathcal{E}(\gamma)_\beta = \emptyset$ for all β
  $\Rightarrow$ micro not realized in Gaussian ensemble

Proof of Theorem 2 from Theorem 1

- Define $P_n^u(d\omega) = P_n(d\omega \mid h_n(\omega) \approx u)$.
- LDP for P_n: $P_n\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI(\nu)}$
- Define $s(u) = -\inf\{I(\nu) : \nu \in \mathcal{X}, f(\nu) = u\}$.

Theorem 1. Relate $\mathcal{E}^u$ and $\mathcal{E}_\beta$ via s.

- Introduce new prior measures

$$P_{n,\gamma}(d\omega) = \text{const} \cdot e^{-n\gamma[h_n(\omega)]^2}\, P_n(d\omega).$$

- Rewrite the Gaussian ensemble:

$$\begin{aligned} P_{n,\beta,\gamma}(d\omega) &= \text{const} \cdot e^{-n\beta h_n(\omega) - n\gamma[h_n(\omega)]^2}\, P_n(d\omega) \\ &= \text{const} \cdot e^{-n\beta h_n(\omega)}\, P_{n,\gamma}(d\omega) \\ &= P_{n,\beta}(d\omega) \text{ with } P_n \text{ replaced by } P_{n,\gamma}. \end{aligned}$$

- Verify $P_n^u(d\omega) \asymp P_{n,\gamma}^u(d\omega)$ since $h_n(\omega) \approx u$.
- Recall $h_n(\omega) = f(L_n(\omega)) + \text{o}(1)$ uniformly over ω.
- LDP for $P_{n,\gamma}$: $P_{n,\gamma}\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-n\left(I(\nu) + \gamma[f(\nu)]^2 - \text{const}\right)}$

Theorem 2. Relate $\mathcal{E}^u$ and $\mathcal{E}(\gamma)_\beta$ via s_γ, where

$$\begin{aligned} s_\gamma(u) &= -\inf\{I(\nu) + \gamma[f(\nu)]^2 : f(\nu) = u\} \\ &= -\inf\{I(\nu) : f(\nu) = u\} - \gamma u^2 \\ &= s(u) - \gamma u^2 \end{aligned}$$

Results for the CWP model

- Prior measure:

$$P_n(\omega) = \frac{1}{q^n} \text{ for each } \omega \in \{1, 2, \ldots, q\}^n$$

- Energy per particle:

$$h_n(\omega) = -\frac{1}{2n^2} \sum_{j,k=1}^n \delta(\omega_j, \omega_k)$$

- Macroscopic variable (empirical vector):

$$L_n = (L_{n,1}, L_{n,2}, \ldots, L_{n,q}),$$
$$L_{n,i}(\omega) = \frac{1}{n} \sum_{j=1}^n 1_i(\omega_j) = \frac{1}{n} \cdot \#\{j : \omega_j = i\}$$

  - Energy representation function:

$$h_n(\omega) = f(L_n(\omega)), \;\; f(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle \text{ for } \nu \in \mathcal{P}(\mathbb{R}^q)$$

  - Basic LDP:

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

    Sanov's Theorem gives rate function

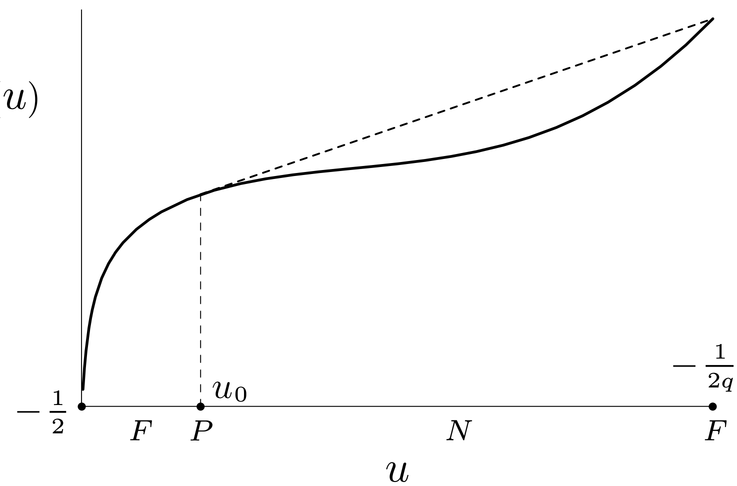
$$R(\nu) = \sum_{i=1}^q \nu_i \log(q\nu_i),$$

    relative entropy of $\sum_{i=1}^q \nu_i \delta_i$ w.r.t. $\sum_{i=1}^q \frac{1}{q}\delta_i$

- Equilibrium macrostates:

$$\mathcal{E}^u = \{\nu \in \mathcal{P}(\mathbb{R}^q) : R(\nu) \text{ is minimized for } f(\nu) = u\}$$
$$\mathcal{E}_\beta = \{\nu \in \mathcal{P}(\mathbb{R}^q) : R(\nu) + \beta f(\nu) \text{ is minimized}\}$$
$$\mathcal{E}(\gamma)_\beta = \{\nu \in \mathcal{P}(\mathbb{R}^q) : R(\nu) + \beta f(\nu) + \gamma[f(\nu)]^2 \text{ is minimized}\}$$

□ $s(u)$ for the Curie-Weiss-Potts Model



$$\text{dom } s = \{u \in \mathbb{R} : s(u) < \infty\} = [-\tfrac{1}{2}, -\tfrac{1}{2q}].$$

Define

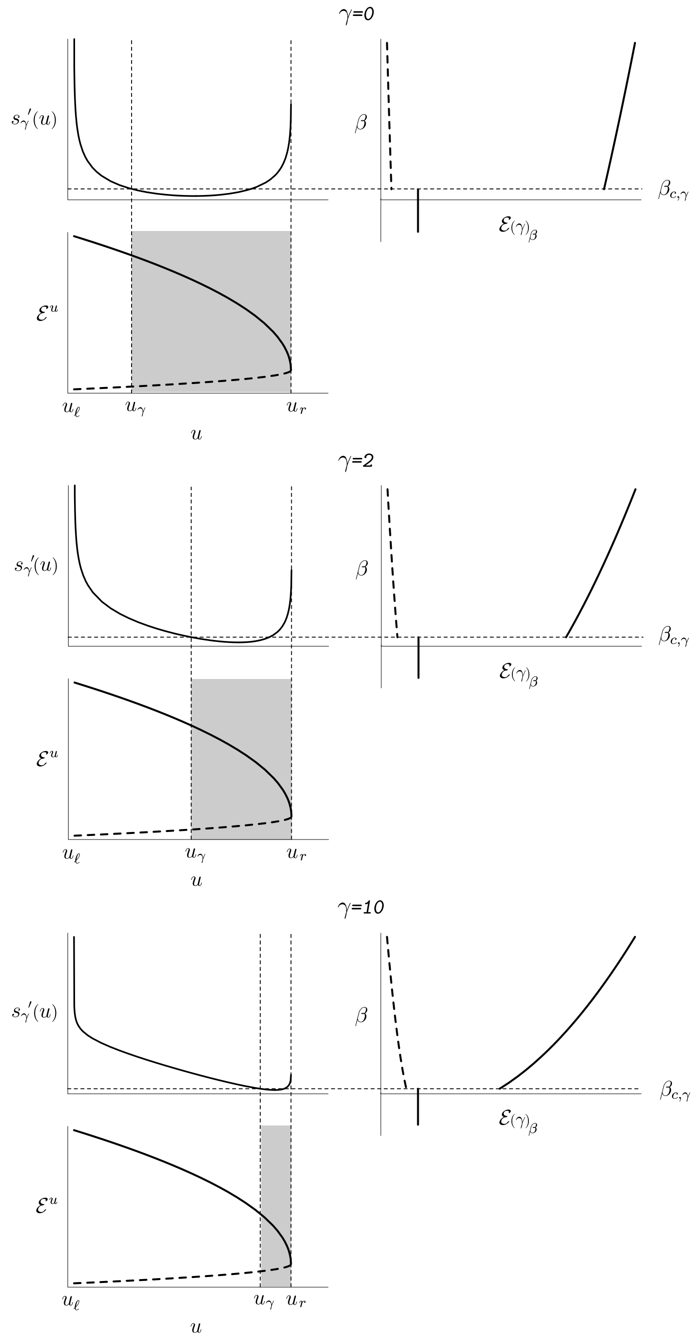
$$\begin{aligned} F &= \{u \in \text{dom } s : \mathcal{E}^u = \mathcal{E}_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ strictly concave at } u\}, \\ P &= \{u \in \text{dom } s : \mathcal{E}^u \subset \mathcal{E}_\beta \text{ but } \mathcal{E}^u \neq \mathcal{E}_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ (not strictly) concave at } u\}, \\ N &= \{u \in \text{dom } s : \mathcal{E}^u \neq \mathcal{E}_\beta \text{ for any } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ not concave at } u\}. \end{aligned}$$

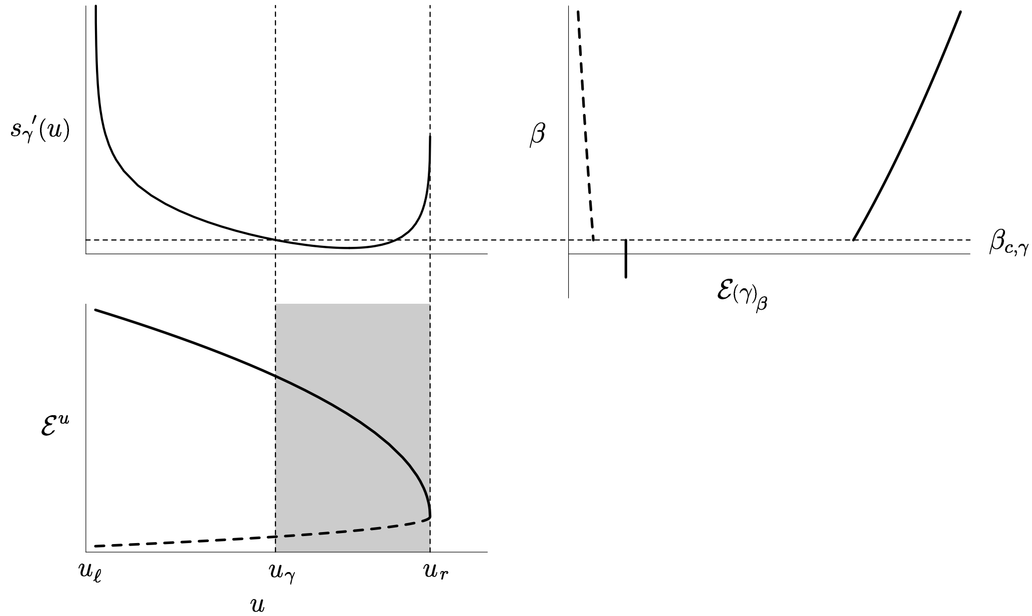
Theorem (*JMP*, 2005). Define $u_0 = \frac{-q^2+3q-3}{2q(q-1)}$. Then

$$\begin{aligned} F &= (-\tfrac{1}{2}, u_0) \cup \{-\tfrac{1}{2q}\}, \\ P &= \{u_0\}, \\ N &= (u_0, -\tfrac{1}{2q}). \end{aligned}$$

□ $\mathcal{E}(\gamma)_\beta$, $(s(u) - \gamma u^2)'$, and $\mathcal{E}^u$ for the CWP Model

- $\mathcal{E}(\gamma)_\beta$ for $\gamma = 0, 2, 10$; $(s(u) - \gamma u^2)'$; and $\mathcal{E}^u$ for $q = 8$
- Full equivalence left of vertical line in $s'(u)$ figure; as $\gamma \uparrow$, full equivalence region increases to $(u_\ell, u_r]$.





$$\text{dom } s = \{u \in \mathbb{R} : s(u) < \infty\} = [u_\ell, u_r] = [-\tfrac{1}{2}, -\tfrac{1}{2q}].$$

For $\gamma \geq 0$ define $s_\gamma(u) = s(u) - \gamma u^2$ and

$$\begin{aligned} F_\gamma &= \{u \in \text{dom } s : \mathcal{E}^u = \mathcal{E}(\gamma)_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s_\gamma \text{ strictly concave at } u\}, \\ P_\gamma &= \{u \in \text{dom } s : \mathcal{E}^u \subset \mathcal{E}(\gamma)_\beta \text{ but } \mathcal{E}^u \neq \mathcal{E}(\gamma)_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s_\gamma \text{ (not strictly) concave at } u\}, \\ N_\gamma &= \{u \in \text{dom } s : \mathcal{E}^u \neq \mathcal{E}(\gamma)_\beta \text{ for any } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s_\gamma \text{ not concave at } u\}. \end{aligned}$$

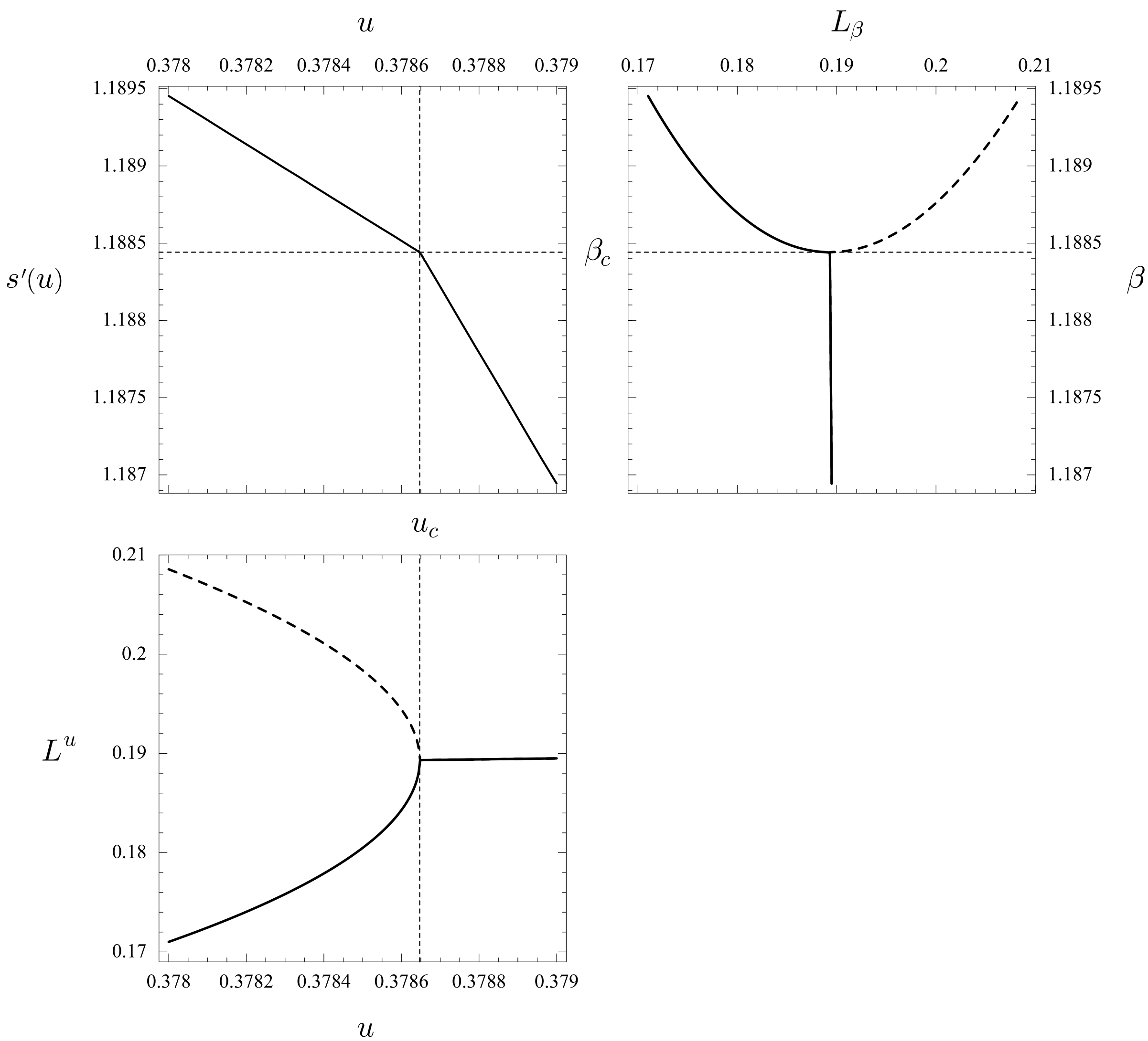
Theorem. There exists $u_\gamma \in (u_\ell, u_r) = (-\frac{1}{2}, -\frac{1}{2q})$ such that

$$F_\gamma = (u_\ell, u_\gamma) \cup \{u_r\},\ P_\gamma = \{u_\gamma\},\ N_\gamma = (u_\gamma, u_r).$$

As $\gamma \to \infty$, $u_\gamma \uparrow u_r$, $F_\gamma \uparrow (u_\ell, u_r]$, and $\beta_{c,\gamma} \to \infty$, where $\beta_{c,\gamma} = s_\gamma'(u_\gamma)$ is the value of β at which $\mathcal{E}(\gamma)_\beta$ has a first-order phase transition.

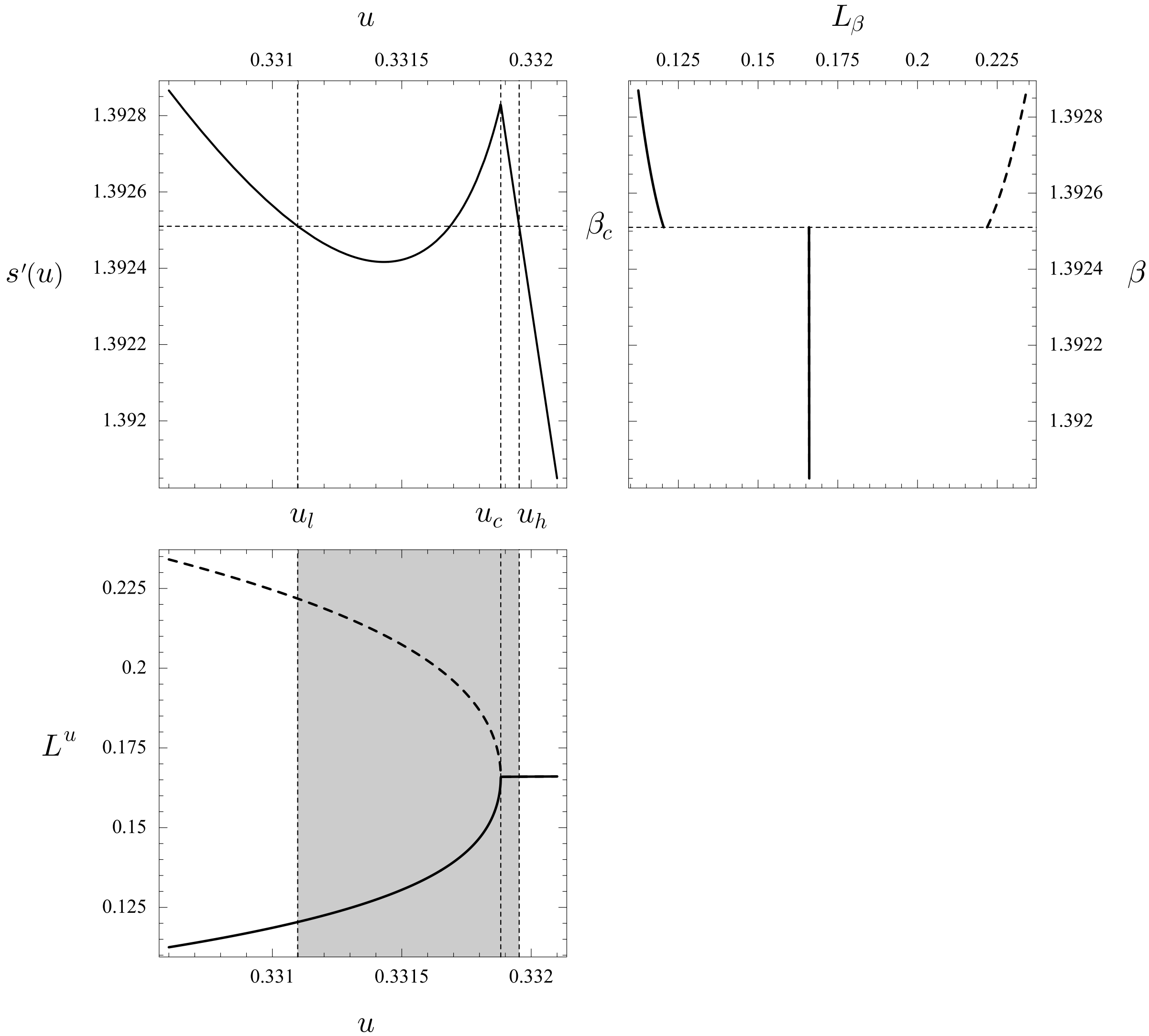
$\mathcal{E}_\beta$, s' , and $\mathcal{E}^u$ for the BEG Model

$K = 1.111111111$ in the mean-field Blume-Emery-Griffiths (BEG) model



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

$K = 1.081651726$ in the mean-field BEG model



- s' not decreasing $\Rightarrow s$ not concave
- $s(u)$ not concave for $u_l = 0.3311 < u < u_h = 0.33195$
- 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

Conclusions and Applications

- Canonical equilibrium macrostates are always realized microcanonically. If s is not strictly concave at u, but $s(u) - \gamma u^2$ is, then the microcanonical equilibrium macrostates not realized canonically are realized in the Gaussian ensemble.

- Universal equivalence of ensembles can be achieved via the Gaussian 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 results generalize to multidimensional cases in which s is a function of energy , enstrophy, circulation, and other quantities conserved by the underlying p.d.e.
  - Apply statistical theories of turbulence to predict 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. Prove their stability via an analysis based on the Gaussian ensemble.

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