# Global Optimization, the Gaussian Ensemble, and Universal Ensemble Equivalence

**Richard S. Ellis**
Department of Mathematics and Statistics
University of Massachusetts Amherst

## Collaborators:

Bruce Turkington, Marius Costeniuc
Department of Mathematics and Statistics
University of Massachusetts Amherst

Kyle Haven
Courant Institute of Mathematical Sciences
New York University

Peter Otto
Department of Mathematics
Union College

Hugo Touchette
School of Mathematical Sciences
Queen Mary University of London

June 2005

---

Research supported by a grant from the National Science Foundation (NSF-DMS-0202309)
Email: `rsellis@math.umass.edu`

# 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 $\beta$, and penalty parameter $\gamma$

- $\mathcal{E}^u =$ 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 $\beta$, $\mathcal{E}_\beta \subset \mathcal{E}^u$ for some $u$
- For fixed $u$
  - $\mathcal{E}^u \subset \mathcal{E}_\beta$ for some $\beta$ (equivalence)
  - $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta$ (nonequivalence)
- If $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta$, can we recover equivalence via the Gaussian ensemble?
  - Want $\beta$ and $\gamma$ 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 $s(u) - \gamma u^2$

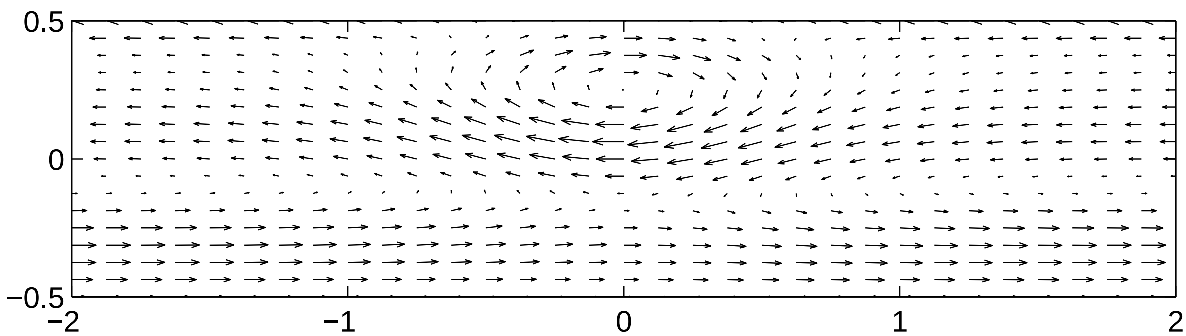
# Statistical Theories of Turbulence

- 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 $\beta$.
- 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 $\beta$:

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

$\beta$ a Lagrange multiplier

3. Unconstrained minimization for given $\beta$, $\gamma$, $u$:

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

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

## Rewrite $\mathcal{E}(\gamma)^u_\beta$

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

- 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)

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

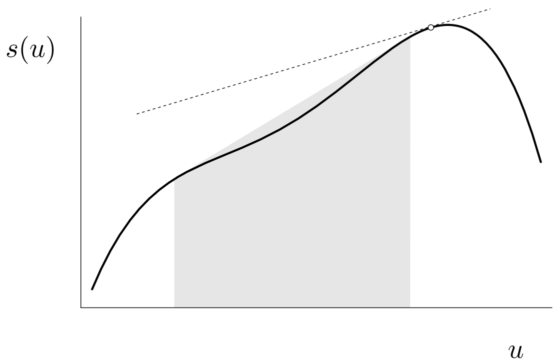
Only 4 relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$.

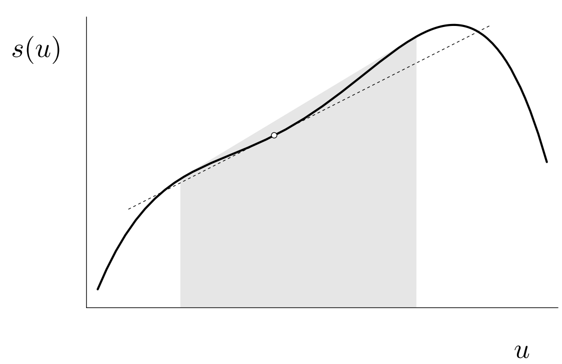
**Theorem** (*JSP*, 2000)

1. Fix $\beta$. Then $\exists u$ such that $\nu \in \mathcal{E}_\beta \Rightarrow \nu \in \mathcal{E}^u$.
2. Fix $u$. Can we always find $\beta$ 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



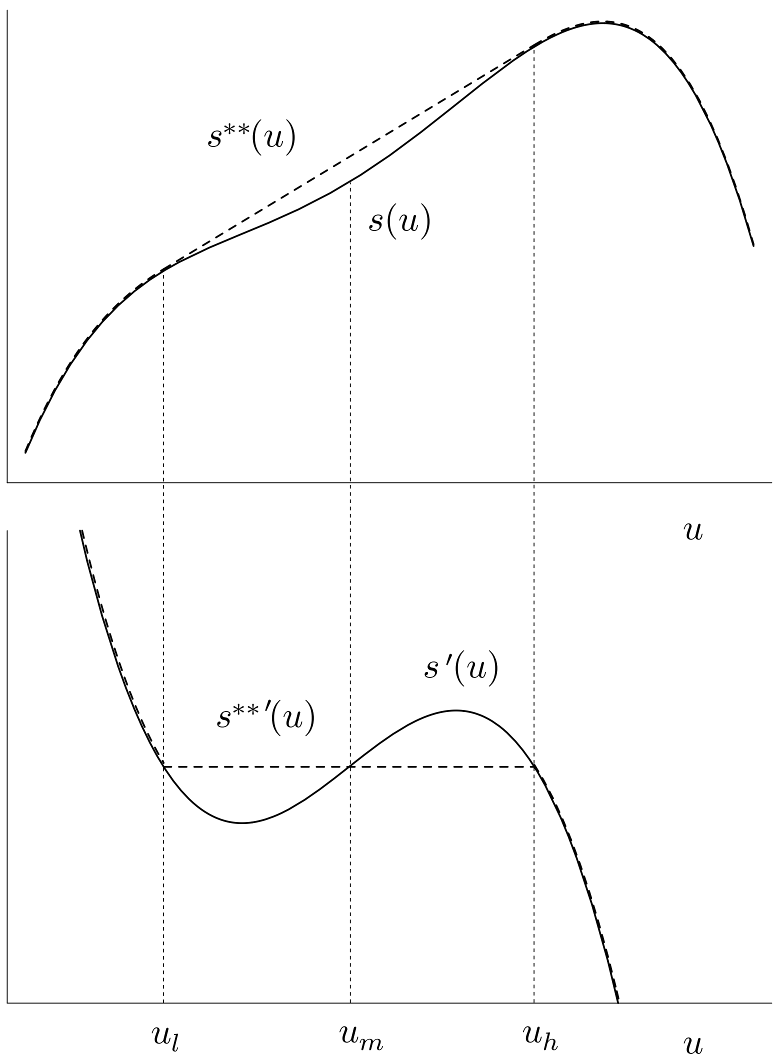

Denote by $u_\ell$ and $u_h$ the projection of the shaded region onto the $u$ axis.

- 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.

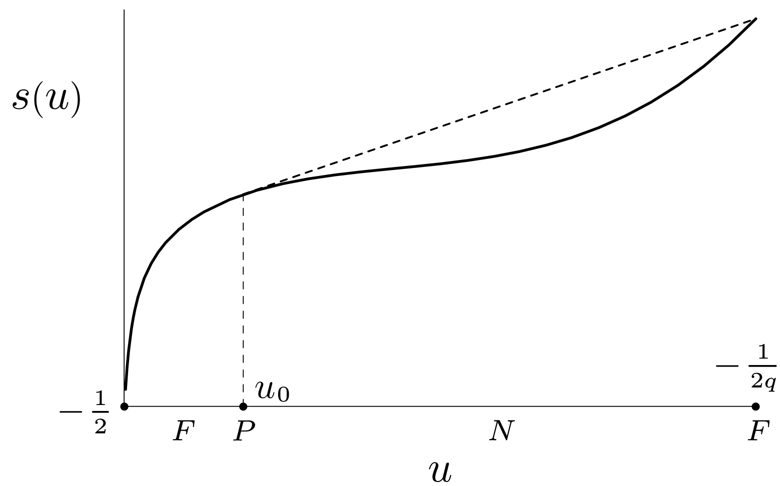
## □ Concave hull $s^{**}$ of $s$

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

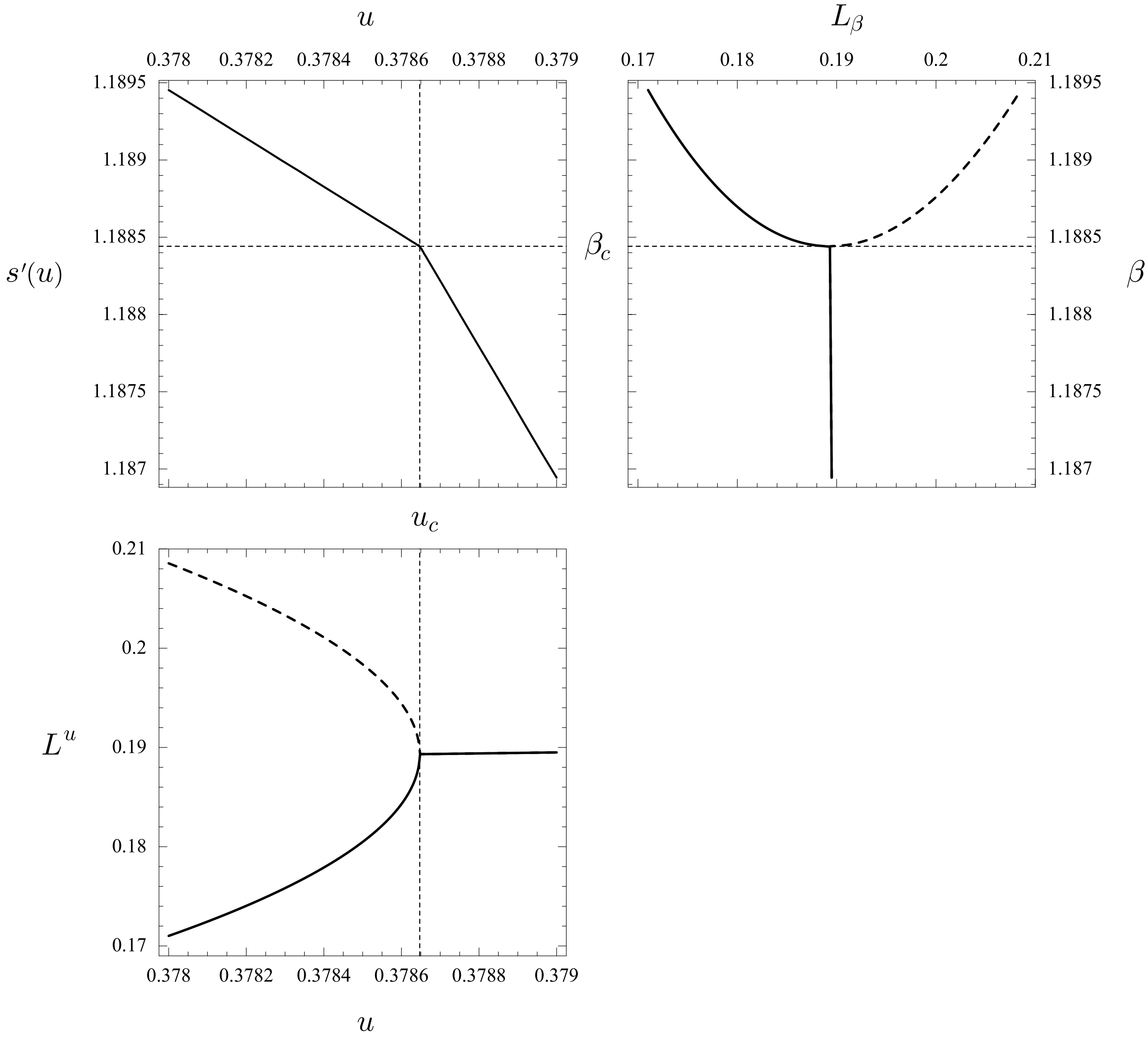
$$\begin{aligned} F &= \{u \in \text{dom } s : \mathcal{E}^u = \mathcal{E}_\beta \text{ for some } \beta \in \mathbb{R}\} \\ &= \{u \in \text{dom } s : s \text{ strictly concave at } u\}, \\ P &= \{u \in \text{dom } s : \mathcal{E}^u \subset \mathcal{E}_\beta \text{ but } \mathcal{E}^u \neq \mathcal{E}_\beta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

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

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

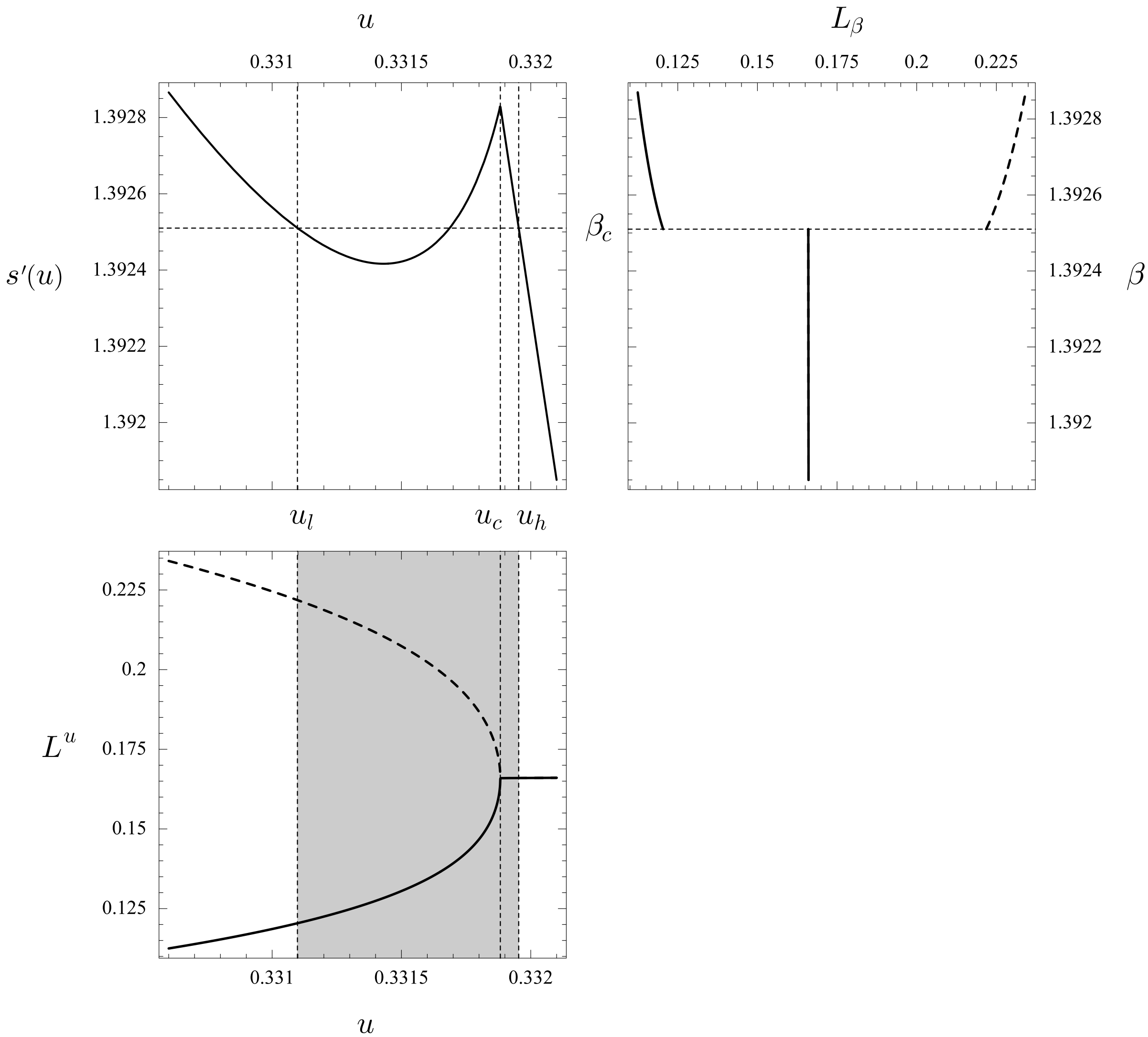
## □ $\mathcal{E}_\beta$ , $s'(u)$, and $\mathcal{E}^u$ for the BEG Model

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




- $s'$ monotonically decreasing $\Rightarrow$ $s$ strictly concave
- Full equivalence of ensembles
- Continuous phase transitions in $\beta$ 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 $\beta_c$ defined by Maxwell-equal-area line
- Nonequivalence of ensembles: for $u_l < u < u_h$ $L^u$ is not realized by $L_\beta$ for any $\beta$: $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta$.
- First-order phase transition in $\beta$ 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 $\beta$ and a subset $A$ of $u$

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

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

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

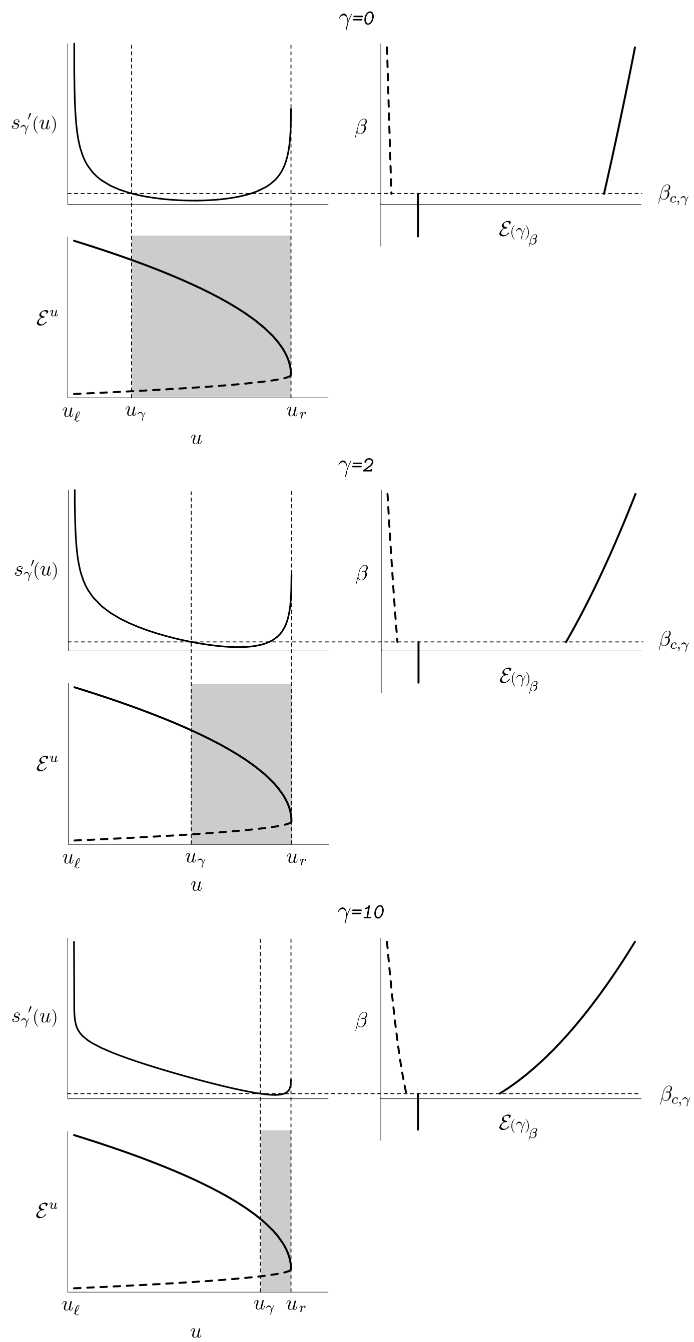
**Surprise.** The simplicity with which $\gamma u^2$ enters the formulation.

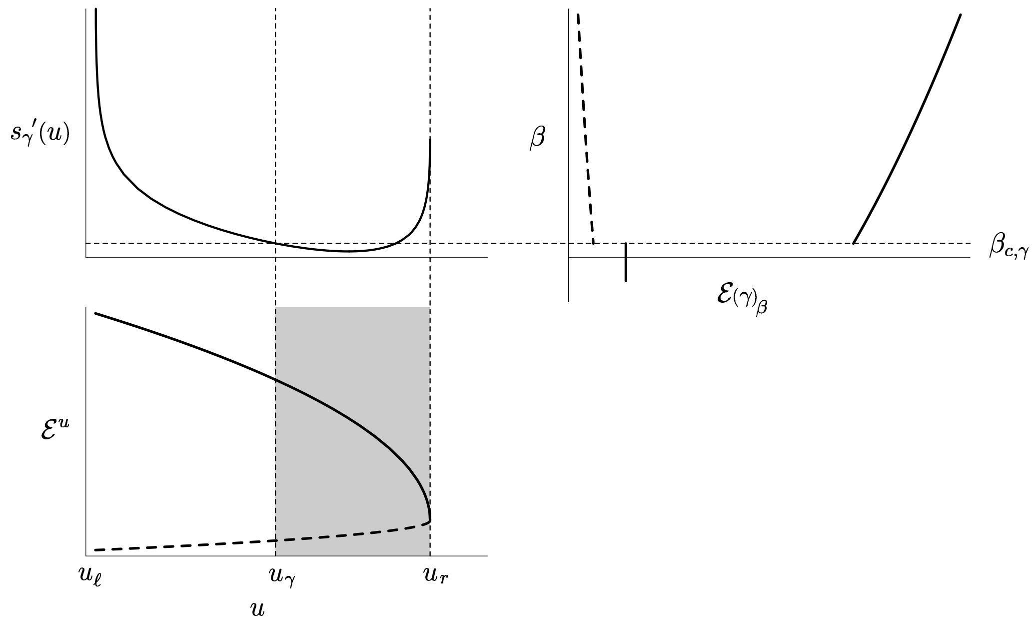
**Theorem.** Define $s(u) = -\inf\{I(\nu) : \nu \in \mathcal{X}, f(\nu) = u\}$.

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 $\beta$ at which $\mathcal{E}(\gamma)_\beta$ has a first-order phase transition.

# Physical Background

Two classical choices of probability distributions in equilibrium statistical mechanics:

**Microcanonical** ensemble

$u = \text{const}$

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

**Canonical** ensemble

$\beta$ or $T = \text{const}$

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. $\omega_i$, $i = 1, 2, \ldots, n$, 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 $\Lambda$ 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 $\Lambda^n$ 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 $n \to \infty$

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

   (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 $\beta$.
    - 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 $\Lambda^n$ into $\mathcal{X}$ such that
  - $h_n(\omega) = f(L_n(\omega)) + \mathrm{o}(1)$ for bdd. cont. $f$: $\mathcal{X} \to \mathbb{R}$
  - $\exists$ 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 $\Lambda$ is a finite set and $P_n(\{\omega\}) = \frac{1}{|\Lambda|^n}$ for each $\omega$, 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 $L_n(\omega)$:

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

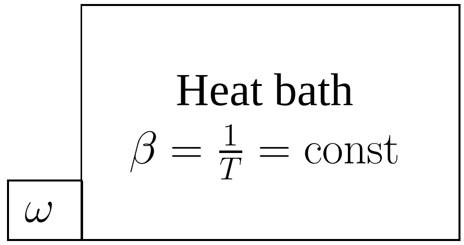
- Microcanonical equilibrium macrostates defined by $I^u(\nu) = 0$:

  $I^u(\nu) \geq 0$ for all $\nu$

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

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

  $\Rightarrow$ canonical $\equiv$ microcanonical

- **Partial equivalence of ensembles:**

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

  $\Rightarrow$ 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 $\beta$

  $\Rightarrow$ Gaussian $\equiv$ microcanonical

  - **Universal equivalence of ensembles**: choose $\gamma$ 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 $\beta$ 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 $\beta$

  $\Rightarrow$ 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 $\omega$.
- 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 $s_\gamma$, 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:

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

  ◦ 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. $\sum_{i=1}^{q} \frac{1}{q} \delta_i$

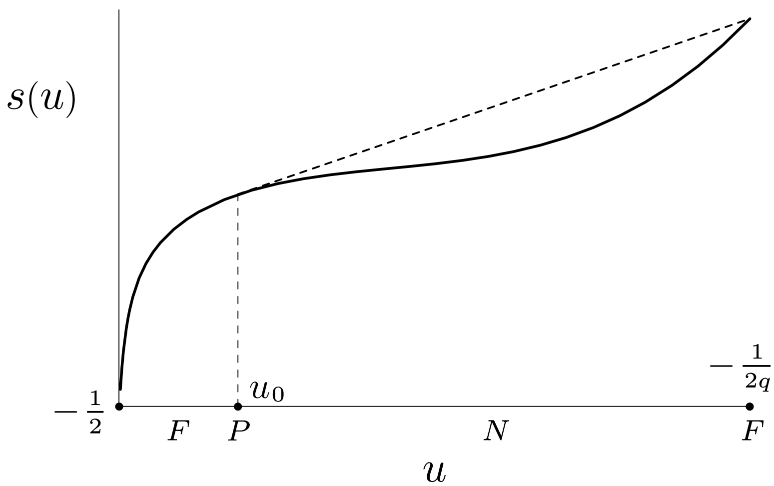
- Equilibrium macrostates:

$$\mathcal{E}^u = \{\nu \in \mathcal{P}(\mathbb{R}^q) : R(\nu) \text{ is minimized for } f(\nu) = u\}$$

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

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

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




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

Define

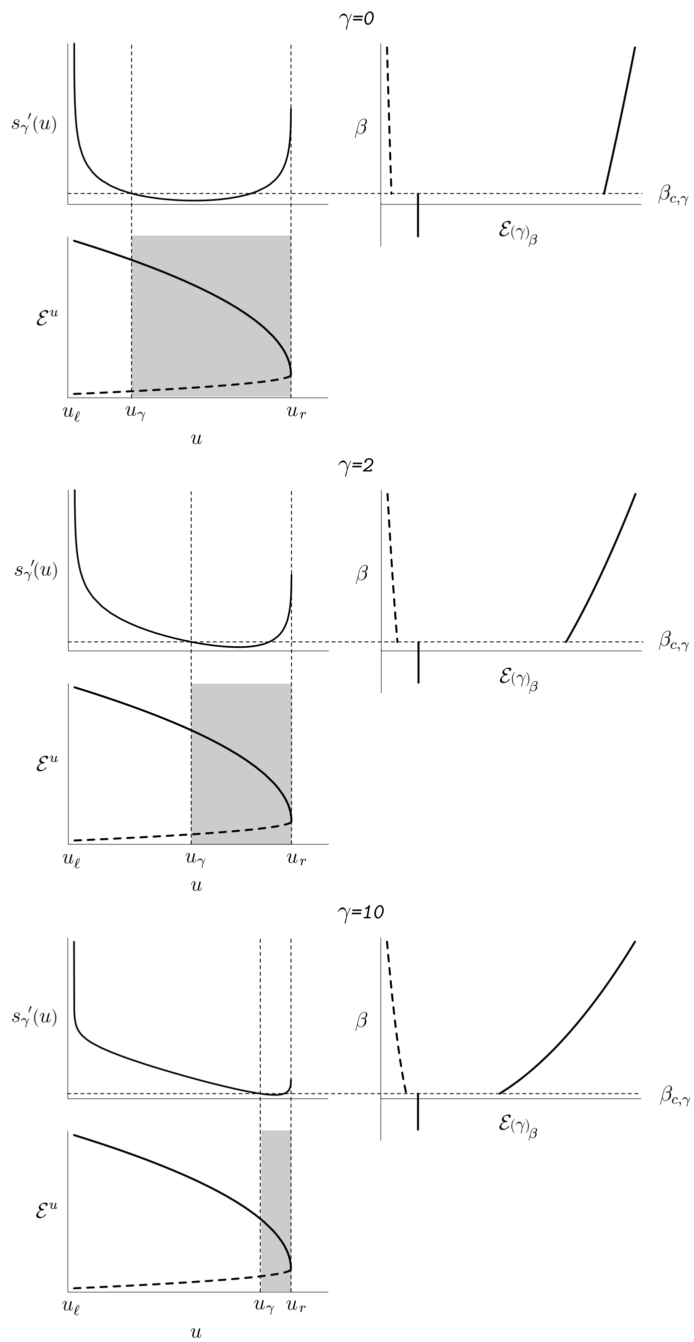
$$\begin{aligned}
F &= \{u \in \text{dom } s : \mathcal{E}^u = \mathcal{E}_\beta \text{ for some } \beta \in \mathbb{R}\} \\
&= \{u \in \text{dom } s : s \text{ strictly concave at } u\}, \\
P &= \{u \in \text{dom } s : \mathcal{E}^u \subset \mathcal{E}_\beta \text{ but } \mathcal{E}^u \neq \mathcal{E}_\beta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

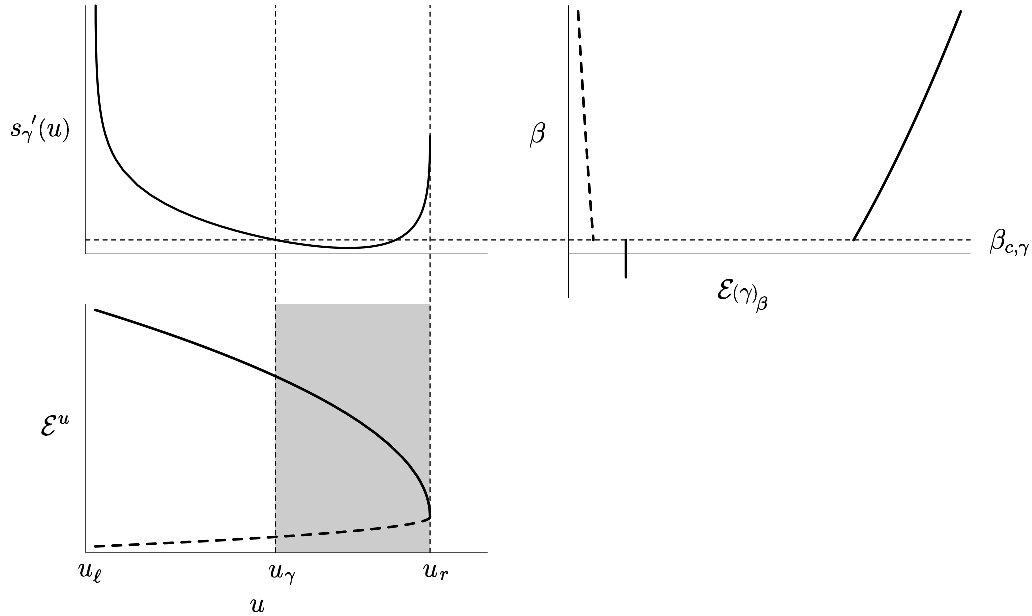
**Theorem** (*JMP*, 2005). Define $u_0 = \frac{-q^2+3q-3}{2q(q-1)}$. Then

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

## □ $\mathcal{E}(\gamma)_\beta$ , $(s(u) - \gamma u^2)'$ , 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

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

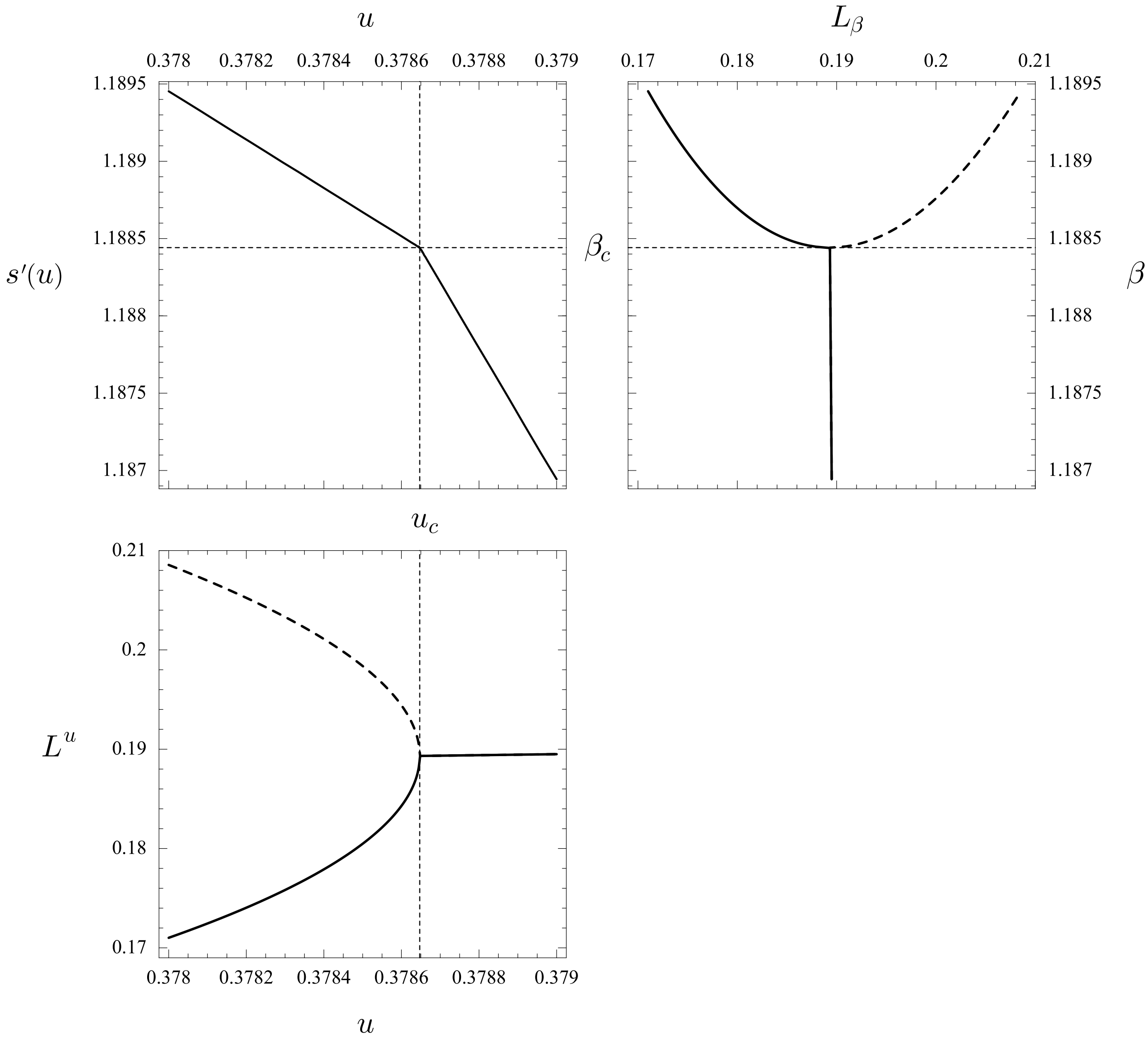
**Theorem**. There exists $u_\gamma \in (u_\ell, u_r) = (-\frac{1}{2}, -\frac{1}{2q})$ such that

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

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 $\beta$ at which $\mathcal{E}(\gamma)_\beta$ has a first-order phase transition.

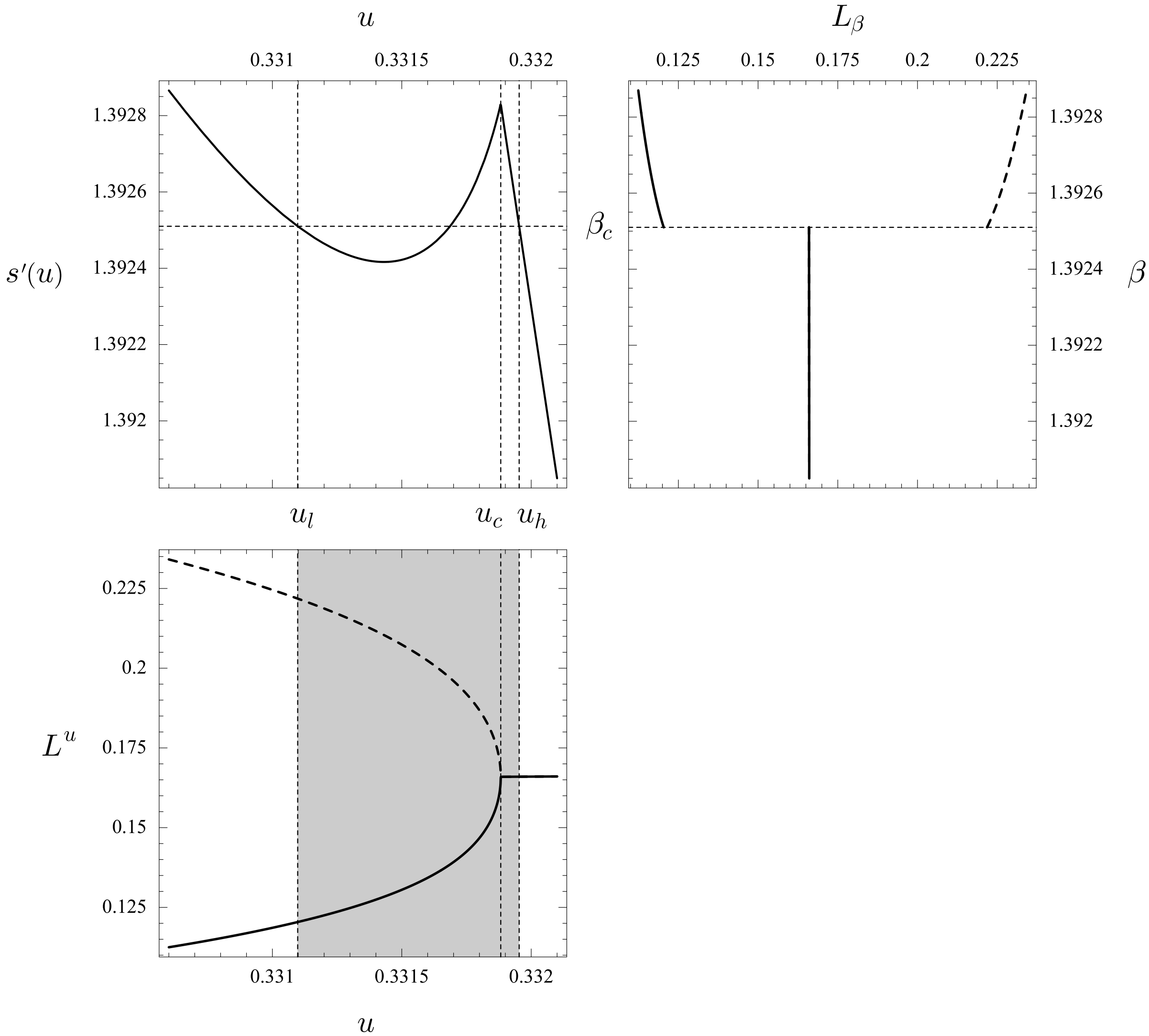
## $\mathcal{E}_\beta$ , $s'$ , and $\mathcal{E}^u$ for the BEG Model

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




- $s'$ monotonically decreasing $\Rightarrow$ $s$ strictly concave
- Full equivalence of ensembles
- Continuous phase transitions in $\beta$ 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 $\beta_c$ defined by Maxwell-equal-area line
- Nonequivalence of ensembles: for $u_l < u < u_h$ $L^u$ is not realized by $L_\beta$ for any $\beta$: $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta$.
- First-order phase transition in $\beta$ 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.

# Bibliography


## Main Reference for This Talk

- M. Costeniuc, R. S. Ellis, H. Touchette, and B. Turkington, "The generalized canonical ensemble and its universal equivalence with the microcanonical ensemble," *J. Stat. Phys.* (2005).

## Blume-Emery-Griffiths Model

- M. Blume, V. J. Emery, R. B. Griffiths, "Ising model for the $\lambda$ transition and phase separation in $He^3$-$He^4$ mixtures," *Phys. Rev. A* **4**: 1071–1077 (1971).

- R. S. Ellis, P. Otto, and H. Touchette. "Analysis of phase transtions in the mean-field Blume-Emery-Griffiths model," *Annals Appl. Prob.* (2005).

## Curie-Weiss-Potts Model

- M. Costeniuc, R. S. Ellis, and H. Touchette, "Complete analysis of equivalence and nonequivalence of ensembles for the Curie-Weiss-Potts model, " *J. Math. Phys.* **46**: 063301 (2005).

- M. Costeniuc, R. S. Ellis, and H. Touchette, “The Gaussian Ensemble and Universal Ensemble Equivalence for the Curie-Weiss-Potts Model,” in preparation.

- R. S. Ellis and K. Wang, ”Limit theorems for the empirical cector of the Curie-Weiss-Potts model,” *Stoch. Proc. Appl.* **35**: 59-79 (1990).


## □ Gaussian Ensemble


- M. S. S. Challa and J. H. Hetherington, “Gaussian ensemble: an alternate Monte-Carlo scheme,” *Phys. Rev. A* **38**: 6324–6337 (1988).

- M. S. S. Challa and J. H. Hetherington, “Gaussian ensemble as an interpolating ensemble,” *Phys. Rev. Lett.* **60**: 77–80 (1988).

  R. S. Johal, A. Planes, and E. Vives, “Statistical mechanics in the extended Gaussian ensemble,” *Phys. Rev. E* **68**: 056113 (2003).


## □ Nonequivalence of Ensembles


- J. Barré, D. Mukamel, S. Ruffo, “Inequivalence of ensembles in a system with long-range interactions,” *Phys. Rev. Lett.* **87**: 030601/1–4 (2001).

- R. S. Ellis, K. Haven, and B. Turkington, "Analysis of statistical equilibrium models of geostrophic turbulence," *J. Appl. Math. Stoch. Anal.* **15**: 341–361 (2002).

- R. S. Ellis, K. Haven, and B. Turkington, "Large deviation principles and complete equivalence and nonequivalence results for pure and mixed ensembles, *J. Stat. Phys.* **101**: 999–1064 (2000).

- R. S. Ellis, K. Haven, and B. Turkington, "Nonequivalent statistical equilibrium ensembles and refined stability theorems for most probable flows," *Nonlinearity* **15**: 239–255 (2002).

- R. S. Ellis, H. Touchette, and B. Turkington, "Thermodynamic versus statistical nonequivalence of ensembles for the mean-field Blume-Emery-Griffiths model, *Physica A* **335**: 518-538 (2004).

- G. L. Eyink and H. Spohn, "Negative-temperature states and large-scale, long-lived vortices in two-dimensional turbulence," *J. Stat. Phys.* **70**: 833–886 (1993).

- M. K.-H. Kiessling and J. L. Lebowitz, "The micro-canonical point vortex ensemble: beyond equivalence," *Lett. Math. Phys.* **42**: 43–56 (1997).

- F. Leyvraz and S. Ruffo, "Ensemble inequivalence in systems with long-range interactions," *J. Math. Phys. A: Math. Gen.* **35**: 285–294 (2002).

- J. T. Lewis, C.-E. Pfister, and W. G. Sullivan, "Entropy, concentration of probability and conditional limit theorems, *Markov Proc. Related Fields* **1**: 319–386 (1995).

- J. T. Lewis, C.-E. Pfister, and W. G. Sullivan, "The equivalence of ensembles for lattice systems: some examples and a counterexample," *J. Stat. Phys.* **77**: 397–419 (1994).

- W. Thirring, *A Course in Mathematical Physics 4: Quantum Mechanics of Large Systems*, trans. E. M. Harrell, New York: Springer-Verlag, 1983.


## □ Theory of Large Deviations


- A. Dembo and O. Zeitouni, *Large Deviations Techniques and Applications*, New York: Springer-Verlag, 1998.

- R. S. Ellis, *Entropy, Large Deviations, and Statistical Mechanics*, New York: Springer-Verlag, 1985.

- R. S. Ellis, "The theory of large deviations: from Boltzmann's 1877 calculation to equilibrium macrostates in 2D turbulence," *Physica D* **133**: 106–136 (1999).

- O. E. Lanford, “Entropy and equilibrium states in classical statistical mechanics,” *Statistical Mechanics and Mathematical Problems* 1–113, ed. A. Lenard, Lecture Notes in Physics, Volume 20, Berlin: Springer-Verlag, 1973.