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

2. Dual minimization without a constraint for $\beta$ given:
   
   Minimize $I(\nu) + \beta f(\nu)$ 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
  
  $$s(u) \doteq -\inf\{I(\nu) : \nu \in \mathcal{X}, f(\nu) = u\}.$$
Physical Motivation

Two choices of probability distributions in equilibrium statistical mechanics:

<table>
<thead>
<tr>
<th>Microcanonical ensemble</th>
<th>Canonical ensemble</th>
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<tbody>
<tr>
<td>$u = \text{const}$</td>
<td>$\beta$ or $T = \text{const}$</td>
</tr>
</tbody>
</table>

- 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., vortices 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)

- $\omega_i$, $i = 1, 2, \ldots, n$, each $\omega_i \in \Lambda$ (spins or vorticities or . . .)
- Microstates: $\omega = (\omega_1, \omega_2, \ldots, \omega_n) \in \Lambda^n$
- 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 $\Lambda$ is a finite set,
  \[ P_n(\{\omega\}) = \frac{1}{|\Lambda|^n} \text{ for each } \omega \]
- 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 . . .).
  - $\mathcal{X}$ is space of macrostates.
  - Require bounded, continuous energy representation function $f$ mapping $\mathcal{X}$ into $\mathbb{R}$: as $n \to \infty$
    \[ h_n(\omega) = f(L_n(\omega)) + o(1) \text{ uniformly over } \omega. \]
  - Require basic LDP with respect to $P_n$:
    \[ P_n\{\omega : L_n(\omega) \approx \nu\} \approx e^{-nI(\nu)}, \]
    $I(\nu)$ rate function for macrostates $\nu \in \mathcal{X}$. 
Example: Curie-Weiss spin model

- $n$ spins $\omega_i \in \{-1, 1\}$
- Microstates: $\omega = (\omega_1, \omega_2, \ldots, \omega_n) \in \{-1, 1\}^n$
- Hamiltonian:
  \[ H_n(\omega) \doteq - \frac{1}{2n} \left( \sum_{i=1}^{n} \omega_i \right)^2 \]
- Energy per particle:
  \[ h_n(\omega) \doteq - \frac{1}{n} H_n(\omega) = - \frac{1}{2} \left( \frac{1}{n} \sum_{i=1}^{n} \omega_i \right)^2 \]
- 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 $f$:
    \[ h_n(\omega) = f(L_n(\omega)), f(\nu) \doteq -\frac{1}{2} \nu^2 \text{ for } \nu \in [-1, 1] \]
  - Basic LDP:
    Cramér’s Theorem: $P_n \{ \omega : \frac{1}{n} \sum_{i=1}^{n} \omega_i \approx \nu \} \asymp e^{-nI(\nu)}$
    \[ I(\nu) \doteq \frac{1-\nu}{2} \log (1 - \nu) + \frac{1+\nu}{2} \log (1 + \nu) \text{ for } \nu \in [-1, 1] \]
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**: \( P_n(\{\omega\}) \overset{\triangle}{=} \frac{1}{|\Lambda|^n} \) for each \( \omega \in \Lambda^n \)

• **Assumption**: \( L_n(\omega) \) maps \( \Lambda^n \) into \( \mathcal{X} \) such that
  
  o \( h_n(\omega) = f(L_n(\omega)) + o(1) \) for bdd. cont. \( f: \mathcal{X} \to \mathbb{R} \)
  
  o \( \exists \) rate function \( I(\nu) \) for macrostates \( \nu \in \mathcal{X} \):
    \[
P_n\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-nI(\nu)}
    \]

**Microcanonical ensemble** \( P^u_n \)

\[
P^u_n(d\omega) = P_n(d\omega \mid h_n(\omega) \approx u)
\]

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

• **Microcanonical entropy** \( s(u) \):

\[
P_n\{\omega : h_n(\omega) \approx u\} \asymp e^{ns(u)}, \quad s(u) \overset{\triangle}{=} -\inf\{I(\nu) : f(\nu) = u\}
\]

\[
P_n\{\omega : h_n(\omega) \approx u\} \approx P_n\{\omega : f(L_n(\omega)) \approx u\}
\]

\[
= P_n\{\omega : L_n(\omega) \in f^{-1}(u)\}
\]

\[
\asymp \sup\{\exp[-nI(\nu) : \nu \in f^{-1}(u)]\}
\]

\[
= \exp[-n \cdot \inf\{I(\nu) : f(\nu) = u\}]
\]

\[
= \exp[-ns(u)]
\]
• Asymptotic $P_n^u$-distribution for $L_n(\omega)$:

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

$$
P_n^u\{\omega : L_n(\omega) \approx \nu\} = P_n\{\omega : L_n(\omega) \approx \nu, h_n(\omega) \approx u\} \cdot \frac{1}{P_n\{\omega : h_n(\omega) \approx u\}}
$$

$$
\approx P_n\{\omega : L_n(\omega) \approx \nu, f(L_n(\omega)) \approx u\} \cdot \frac{1}{P_n\{\omega : h_n(\omega) \approx u\}}
$$

$$
= P_n\{\omega : L_n(\omega) \approx \nu\} \cdot \frac{1}{P_n\{\omega : h_n(\omega) \approx u\}} \approx \exp[-n(I(\nu) + s(u))].
$$

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

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

$$
P_n^u\{\omega : L_n(\omega) \approx \nu\} \approx e^{-nI_u(\nu)}
$$

$$
I_u(\nu) = \left\{
\begin{array}{ll}
I(\nu) + s(u) & \text{if } f(\nu) = u \\
\infty & \text{otherwise}
\end{array}
\right.
$$

• Microcanonical equilibrium macrostates defined by $I_u(\nu) = 0$:

$I_u(\nu) \geq 0$ for all $\nu$

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

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

$$
\mathcal{E}^u = \{\nu \in \mathcal{X} : I(\nu) \text{ is minimized for } f(\nu) = u\}
$$
**Canonical ensemble** $P_{n,\beta}$

- **Heat bath**
  
  $\beta = \frac{1}{T} = \text{const}$

- 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 $L_n(\omega)$:

  $P_{n,\beta}\{\omega : L_n(\omega) \approx \nu\} \asymp e^{-n I_\beta(\nu)}$

  $I_\beta(\nu) \doteq I(\nu) + \beta f(\nu) - \varphi(\beta)$

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

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

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

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

  $\mathcal{E}^u = \{\nu \in \mathcal{X} : I(\nu) \text{ is minimized for } f(\nu) = u\}$
Nonequivalence of ensembles: thermodynamic point of view

- 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 $\varphi$ is Legendre-Fenchel transform of entropy $s$:
  \[
  Z_n(\beta) = \int_{\mathbb{R}} e^{-\beta n u} P_n\{\omega : h_n(\omega) \in du\}
  \asymp \int_{\mathbb{R}} e^{-\beta n u} e^{ns(u)} du \asymp \exp \left[ -n \cdot \inf_u \left\{ \beta u - s(u) \right\} \right]
  \]
  \[
  \varphi(\beta) = \inf_u \left\{ \beta u - s(u) \right\} = s^*(\beta)
  \]

- Inversion of Legendre-Fenchel transform:
  \[
  s(u) \doteq \inf_{\beta} \left\{ \beta u - \varphi(\beta) \right\} = \varphi^*(u)
  \]
  - Equality if $s(u)$ is concave or $\varphi(\beta)$ differentiable
    * Thermodynamic equivalence of ensembles
  - $\varphi(\beta)$ is always concave.
• Concave hull $s^{**}(u)$ of $s(u)$:

$$
\begin{align*}
  s^{**}(u) & := \inf_{\beta} \{ \beta u - s^*(\beta) \} = \inf_{\beta} \{ \beta u - \varphi(\beta) \} \\
  \varphi(\beta) & = \inf_u \{ \beta u - s(u) \} = \inf_u \{ \beta u - s^{**}(u) \}
\end{align*}
$$

• **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

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

This implies

\[
\varphi(\beta) \doteq -\frac{1}{n} \log Z_n(\beta) = \inf_u \{\beta u - s(u)\}.
\]

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 \( \varphi \) (complicated)

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

- \( \varphi(\beta) \) not differentiable \( \implies \)

  - 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

<table>
<thead>
<tr>
<th>Properties of microcanonical equilibrium macrostates</th>
<th>Properties of canonical equilibrium macrostates</th>
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- 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 \( \beta \) 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

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

Macrostate equivalence $\iff$ thermodynamic equivalence

![Diagram showing microcanonical entropy and canonical free energy curves with critical points $u_i, u_m, u_h$]
\textbf{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 $s(u) \neq s^{**}(u)$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{concave_hull.png}
\caption{Concave hull of $s$}
\end{figure}
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:**
  \[ s(u) \doteq -\inf\{I(\nu) : f(\nu) = u\} \text{ strictly concave at } u \]
  \[ \implies \mathcal{E}^u = \mathcal{E}_\beta \text{ for unique } \beta \]
  \[ \implies \text{canonical } \equiv \text{ microcanonical} \]

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

- **Partial equivalence of ensembles:**
  \[ s(u) \text{ (not strictly) concave at } u \implies \mathcal{E}^u \subsetneq \mathcal{E}_\beta \text{ for unique } \beta \]

- **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 microcannically. 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: $\omega = (\omega_1, \omega_2, \ldots, \omega_n) \in \{-1, 0, 1\}^n$
- Hamiltonian:
  \[
  H_n(\omega) = \sum_{i=1}^{n} \omega_i^2 - \frac{K}{n} (\sum_{i=1}^{n} \omega_i)^2
  = \left( N_{n,1} + N_{n,-1} \right) - \frac{K}{n} (N_{n,1} - N_{n,-1})^2,
  \]
  \[
  N_{n,j} = \sum_{i=1}^{n} 1_j \{\omega_i\} = \# \{i : \omega_i = j\}
  \]
- Energy per particle:
  \[
  h_n(\omega) = \frac{1}{n} H_n(\omega) = L_{n,1} + L_{n,-1} - K (L_{n,1} - L_{n,-1})^2
  \]
- Macroscopic variable (empirical vector):
  \[
  L_n = (L_{n,-1}, L_{n,0}, L_{n,1}),
  \]
  \[
  L_{n,j}(\omega) = \frac{1}{n} \sum_{i=1}^{n} 1_j (\omega_i) = \frac{1}{n} \cdot \# \{i : \omega_i = j\},
  \]
  \[
  L_{n,j} \geq 0, L_{n,-1} + L_{n,0} + L_{n,1} = 1 \implies L_n(\omega) \in \mathcal{P}(\{-1, 0, 1\})
  \]
- A priori measure:
  \[
  P_n(\omega) = \frac{1}{3^n} \text{ for each } \omega
Large deviation analysis of the mean-field BEG model

- A priori measure:
  \[ P_n(\omega) = \frac{1}{3^n} \text{ for each } \omega \]

- Energy per particle:
  \[ h_n(\omega) = L_{n,1} + L_{n,-1} - K(L_{n,1} - L_{n,-1})^2 \]

- Macroscopic variable (empirical vector):
  \[ L_n = (L_{n,-1}, L_{n,0}, L_{n,1}), \]
  \[ L_{n,j}(\omega) = \frac{1}{n} \sum_{i=1}^{n} 1_j(\omega_i) = \frac{1}{n} \# \{ i : \omega_i = j \} \]
  - Energy representation function:
    \[ h_n(\omega) = f(L_n(\omega)), \quad f(\nu) = \nu_1 + \nu_{-1} - K(\nu_1 - \nu_{-1})^2 \]
    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
\[ R(\nu) = \nu_{-1} \log(3\nu_{-1}) + \nu_0 \log(3\nu_0) + \nu_1 \log(3\nu_1), \]
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:
  \[ L_u = \arg \inf_{\nu} \{ R(\nu) : f(\nu) = u \} \]
  \[ L_\beta = \arg \inf_{\nu} \{ R(\nu) + \beta f(\nu) \} \]
Exact comparison of equilibrium macrostates

\[ s(u) \doteq -\inf\left\{ R(\nu) : \nu_1 + \nu_{-1} - K(\nu_1 - \nu_{-1})^2 = u \right\} \]

\[ K = 1.11111111 \]

- \( s' \) monotonically decreasing \( \Rightarrow \) \( s \) strictly concave
- Complete equivalence of ensembles
- Continuous phase transitions in \( \beta \) 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 $\beta_c$ 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 $u$
\[ K = 1.080501698 \]

- \( s' \) 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 \( \beta_c \) given 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 transitions in \( \beta \) and \( u \)
\[ K = 1.050001050 \]

- Similar features as on preceding transparency: nonequivalence of ensembles and first-order phase transitions in \( \beta \) 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 ≠ 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).
Bibliography

Theory of Large Deviations


BEG Model

Nonequivalence of Ensembles


