Nonconcave entropies from generalized canonical ensembles

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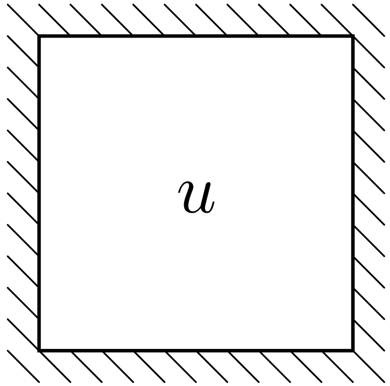
Support from NSERC (Canada) and the
Royal Society of London

Queen Mary
University of London

■ Context — plan

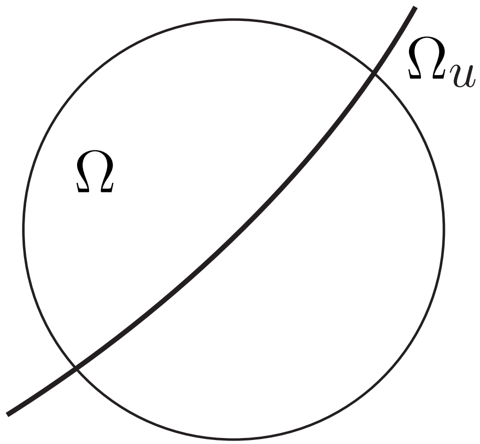
- Long-range systems have special properties
  - Their entropy can be nonconcave
- Nonconcavity breaks the Legendre transform of thermodynamics
  - Entropy $\neq$ Legendre transform of canonical free energy
- How to calculate a nonconcave entropy?
  - Revision of concepts
  - Problem with nonconcave entropies
  - Generalized canonical ensemble
  - Example

■ Equilibrium statistical mechanics



- Microstate: $\omega \in \Omega$
- Hamiltonian: $U(\omega)$
- Mean energy: $u = U/n$

□ Microcanonical ensemble



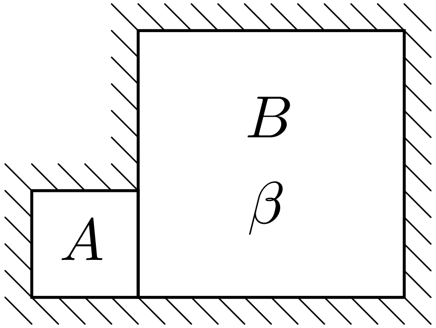
- Density of states:

$$\rho(u) = \int_{\Omega_u} d\omega = \int_{\Omega} \delta(u(\omega) - u)\, d\omega$$

- **Entropy function:**

$$s(u) = \lim_{n\to\infty} \frac{1}{n} \log \rho(u)$$

□ Canonical ensemble



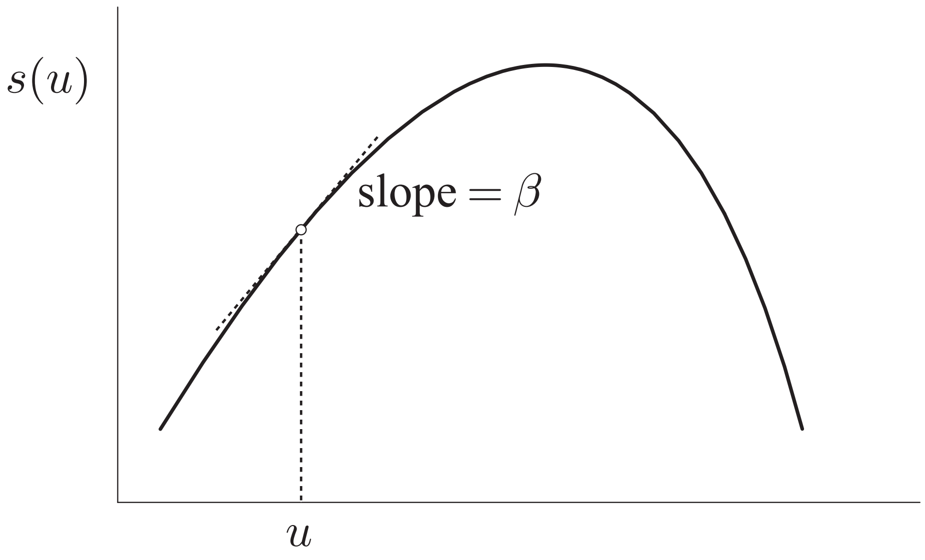
- Partition function:

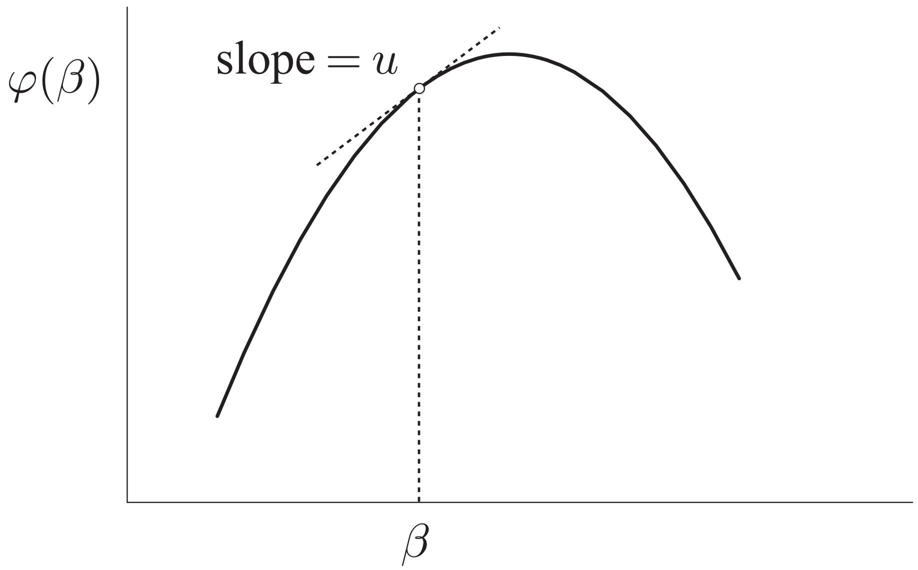
$$Z(\beta) = \int_\Omega e^{-\beta U(\omega)}\, d\omega$$

- **Free energy function:**

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

■ Calculation of the entropy function





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

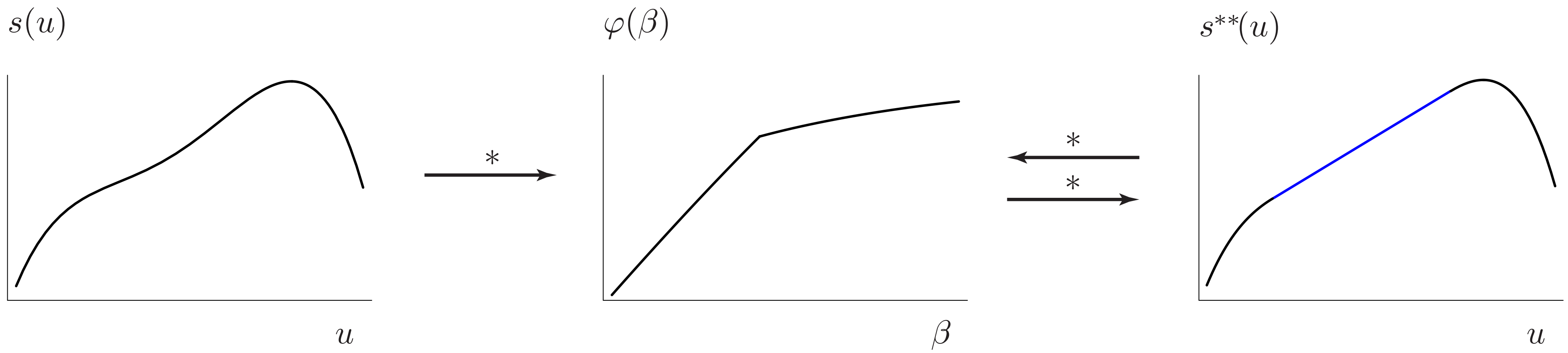
$$\varphi'(\beta) = u \qquad s'(u) = \beta$$

$$s \longleftrightarrow \varphi$$

$$u \longleftrightarrow \beta$$

$$s = \varphi^* \qquad \varphi = s^*$$

Problem with nonconcave entropies



Nonconcave

s

Always concave

$\varphi = s^*$

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

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

- $s^{**}(u)$ is the concave envelope of $s(u)$
- $s^{**}(u) \geq s(u)$

■ Systems with nonconcave entropies

- Gravitating systems
- Spin models
  - Hamiltonian mean-field model
  - Blume-Emery-Griffiths model
  - Potts model
- 2D turbulence models
- String theory
- Multifractals
- Thermodynamic formalism of chaotic systems

■ Generalized canonical ensembles

Costeniuc, Ellis, Touchette & Turkington
JSP **119**, 1283 (2005); PRE **73**, 026105 (2006)

□ Definition

Standard canonical

$$P_\beta = \frac{e^{-n\beta u}}{Z(\beta)}$$

$$Z(\beta) = \sum_{\text{microstates}} e^{-n\beta u}$$

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

Generalized canonical

$$P_g = \frac{e^{-n\alpha u - n g(u)}}{Z_g(\alpha)}$$

$$Z_g(\alpha) = \sum_{\text{microstates}} e^{-n\alpha u - n g(u)}$$

$$\varphi_g(\alpha) = -\lim_{n\to\infty} \frac{1}{n} \log Z_g(\alpha)$$

□ Calculation of the entropy

- Concave entropy:

$$s = \varphi^*$$

- Nonconcave entropy:

$$s \neq \varphi^*$$

- Modified Legendre transform:

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

Theorem

If, for a given g, $\varphi_g(\alpha)$ is differentiable at α, then

$$s(u) = \alpha u - \varphi_g(\alpha) + g(u), \qquad \varphi_g'(\alpha) = u$$

■ Example: The 3-state mean-field Potts model

□ Definition of the model

- Microstate: $\omega = \omega_1, \omega_2, \ldots, \omega_n, \quad \omega_i \in \{1, 2, 3\}$
- Hamiltonian:

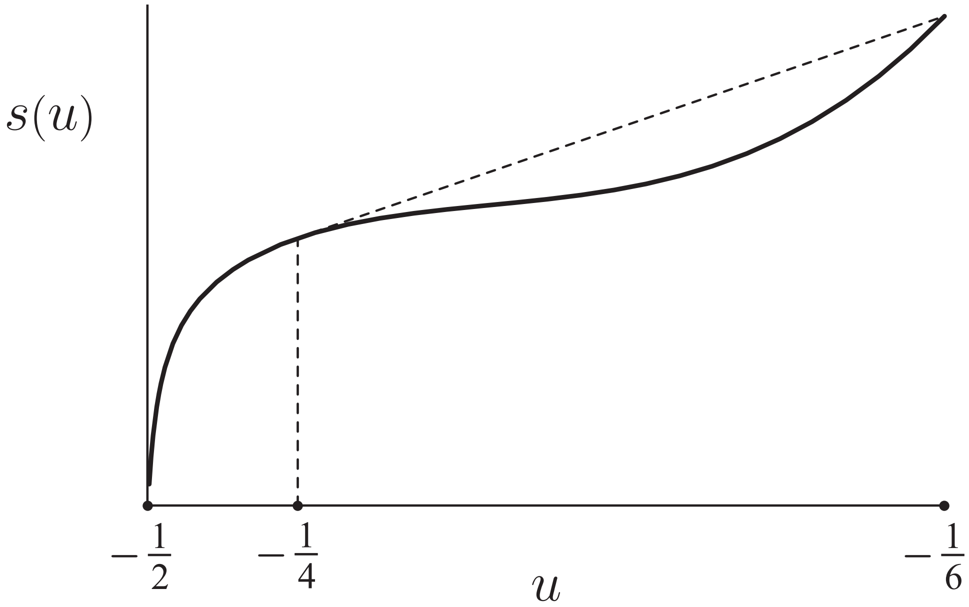
$$U(\omega) = -\frac{1}{2n} \sum_{i,k=1}^{n} \delta(\omega_i, \omega_k)$$

- Energy per spin:

$$u = \frac{U}{n} = -\frac{1}{2}(\nu_1^2 + \nu_2^2 + \nu_3^2), \qquad \nu_i = \frac{\text{\# spins } i}{n}$$

□ Entropy function

Costeniuc, Ellis & Touchette, J. Math. Phys. **46**, 063301, 2005



$$s(u) = -\frac{1+\sqrt{2(-6u-1)}}{3}\log\left(1+\sqrt{2(-6u-1)}\right) - \frac{2-\sqrt{2(-6u-1)}}{3}\log\left(\frac{2-\sqrt{2(-6u-1)}}{2}\right)$$

□ Gaussian ensemble

- g-function:

$$g(u) = \frac{\gamma}{2}u^2, \qquad \gamma \in \mathbb{R}$$

- Partition function:

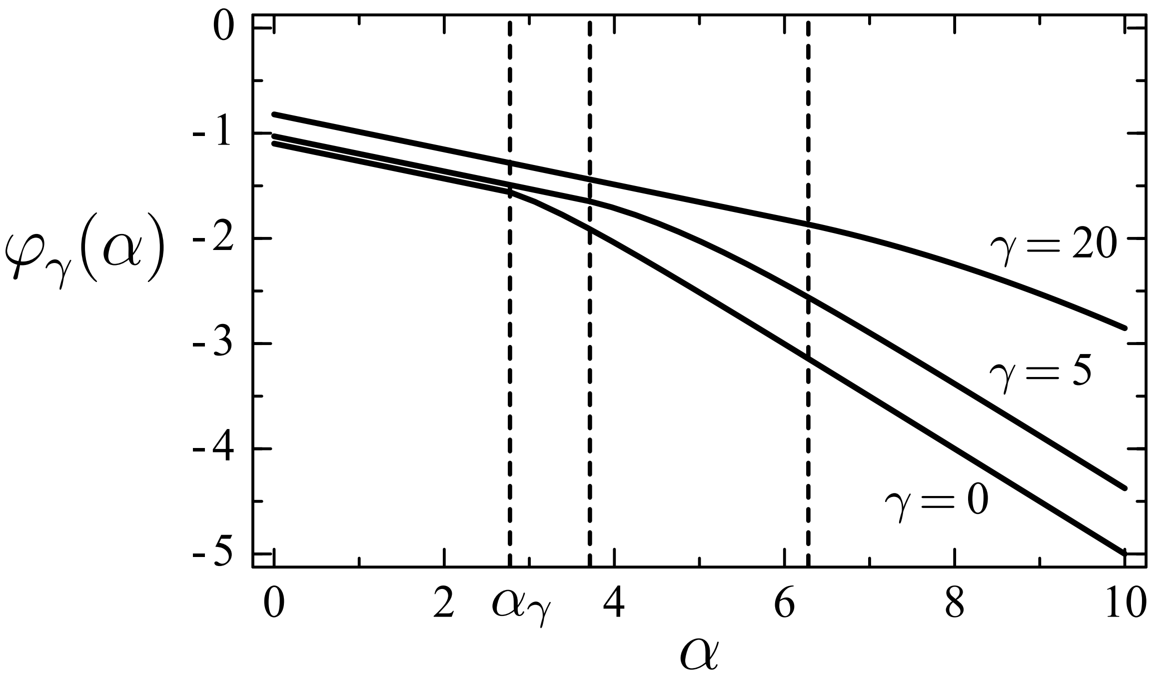
$$Z_\gamma(\alpha) = \sum_{\text{microstates}} e^{-n\alpha u - n\gamma u^2/2}, \qquad \alpha, \gamma \in \mathbb{R}$$

- Free energy:

$$\varphi_\gamma(\alpha) = -\lim_{n\to\infty} \frac{1}{n} \log Z_\gamma(\alpha)$$

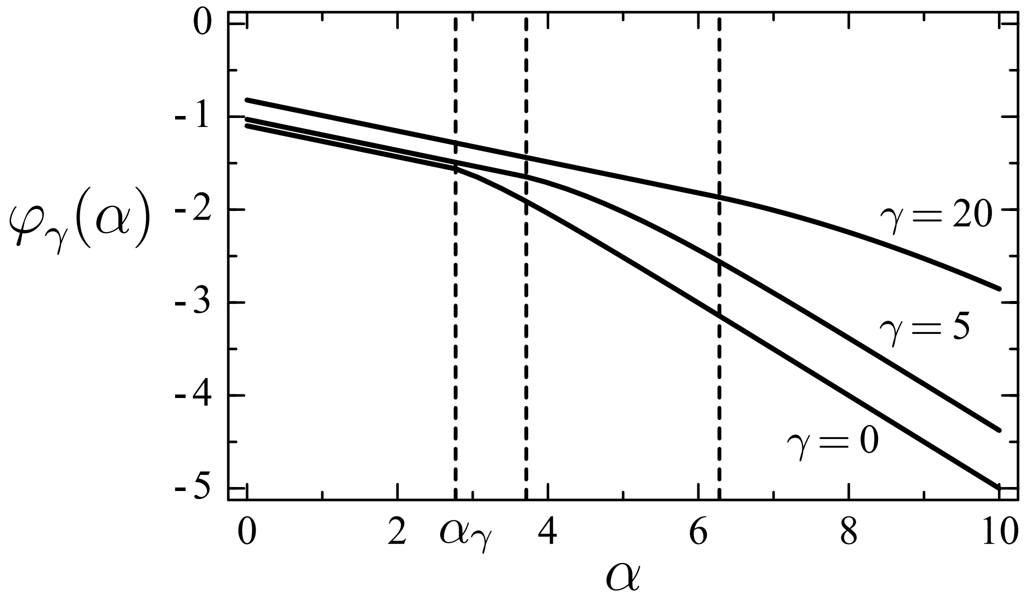
□ Calculation of the Gaussian free energy

Costeniuc, Ellis & Touchette, `cond-mat/0605213`, to appear in PRE

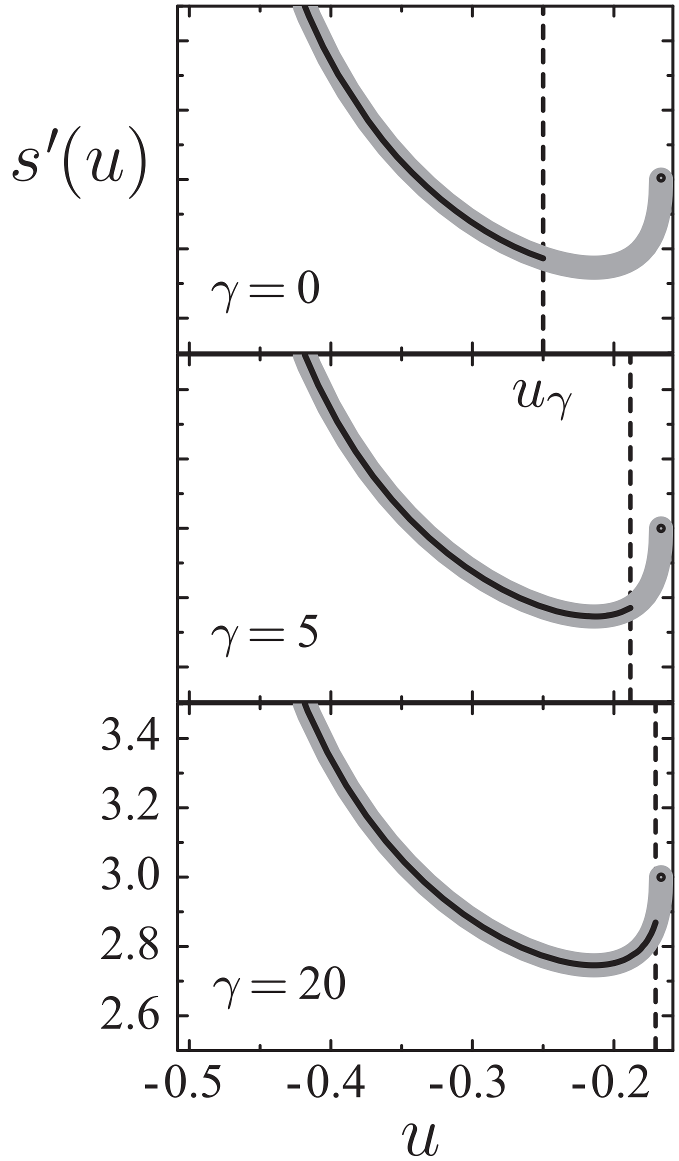


- Non-differentiable point: α_γ
- Left branch: $\varphi'_\gamma(\alpha) = -\frac{1}{6}$
- Right branch: $\varphi'_\gamma(\alpha) \in (-\frac{1}{2}, u_\gamma)$

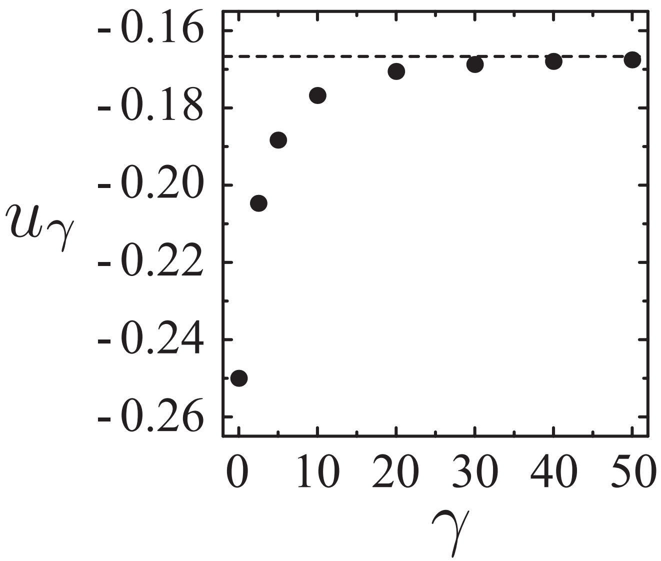
□ Calculation of the entropy

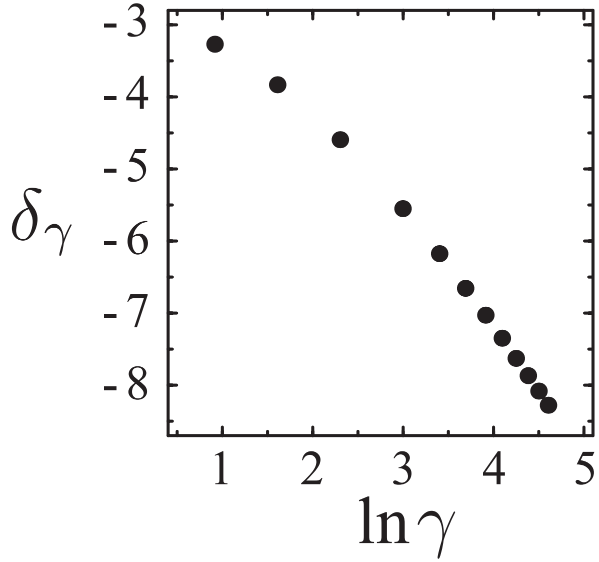


- $s = \varphi_g^* + g$
- $s(u) = \alpha u + \frac{\gamma}{2}u^2 - \varphi_\gamma(\alpha)$
- $u = \varphi'_\gamma(\alpha) \in (-1/2, u_\gamma)$



□ Asymptotic equivalence





- Maximum mean energy: $u_\gamma = \varphi'_\gamma(\alpha_\gamma + 0)$
- Asymptotic limit:

$$u_\gamma \to u_{\mathrm{max}} = -\frac{1}{6} \quad \text{as} \quad \gamma \to \infty$$

- Scaling:

$$\delta_\gamma = \ln |u_\gamma - u_{\mathrm{max}}| \sim -2 \ln \gamma$$

□ Equivalence at the macrostate level

- Macrostate:

$$a = \frac{\#\text{ spin } 1}{n}$$

- Gaussian equilibrium:

$$a_{\gamma,\alpha}$$

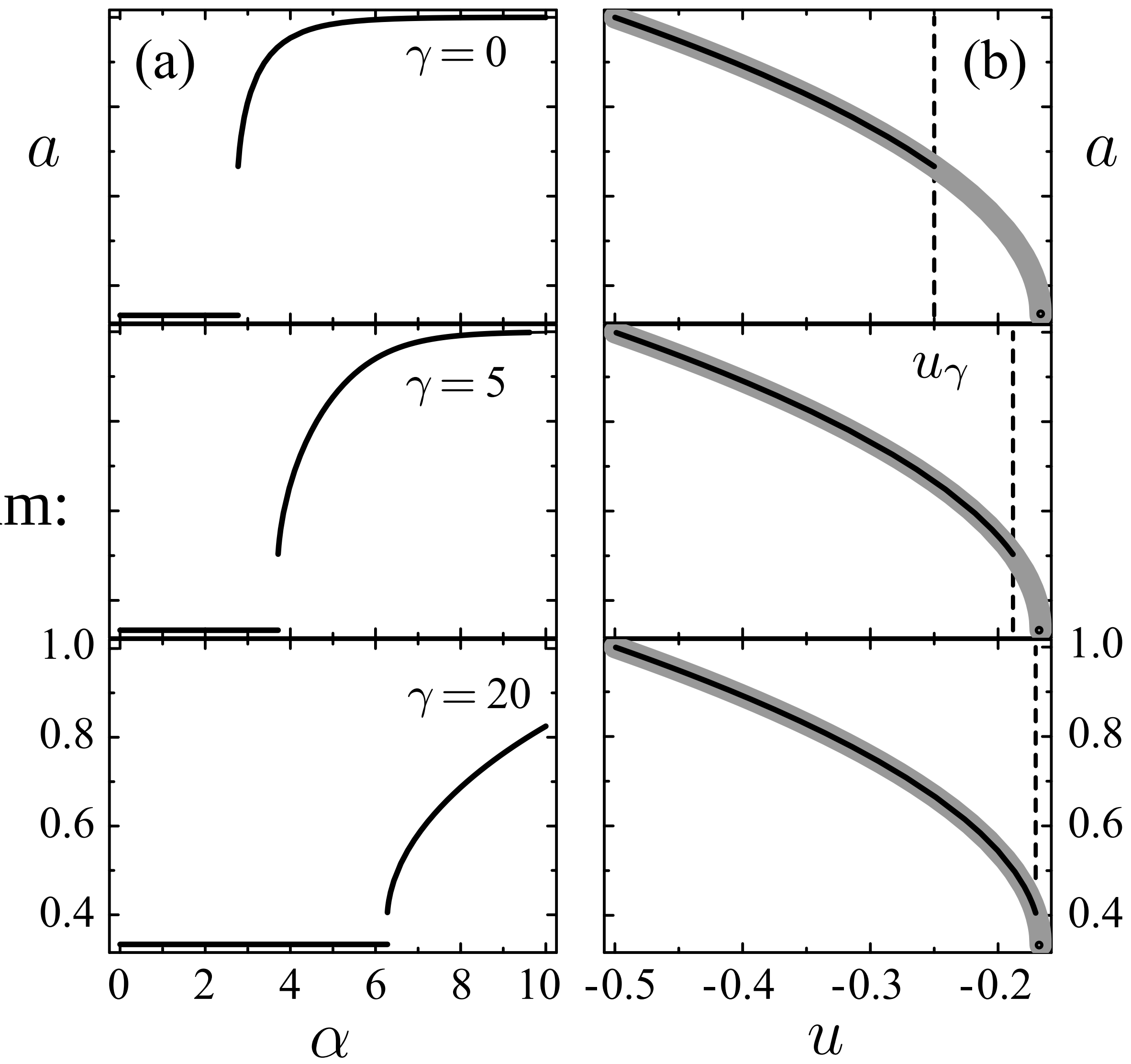
- Microcanonical equilibrium:

$$a^u$$

  - ○ $a^{-\frac{1}{2}} = 1$
  - ○ $a^{-\frac{1}{6}} = \frac{1}{3}$

- Mapping:

$$a \rightarrow (u(a), a)$$



■ Summary

- Entropy can be **nonconcave** (for long-range systems)
- Related to first-order phase transitions
- Nonconcave entropies cannot be calculated in the canonical ensemble

$$s \neq \varphi^*$$

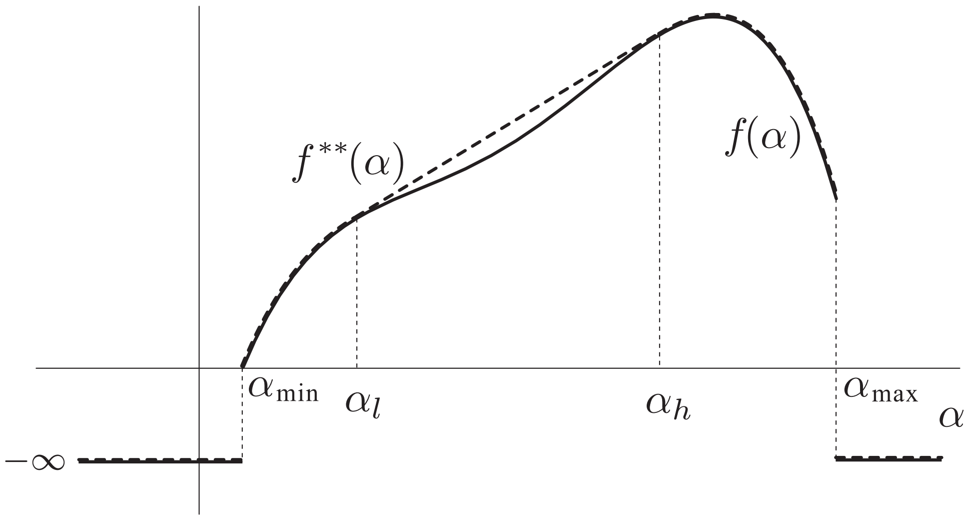
- Fix the problem: generalized canonical ensembles

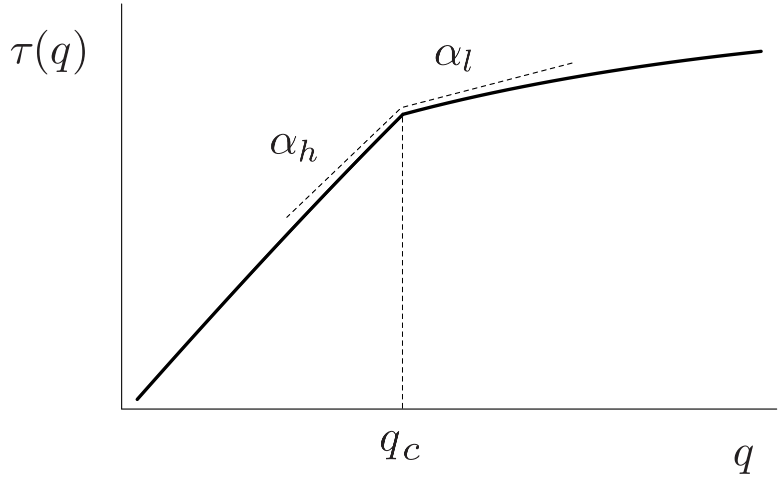
$$s = \varphi_g^* + g$$

- Gaussian ensemble: $g(u) = \gamma u^2$
  - **Any** shape of entropy can be obtained via the Gaussian ensemble
  - Gaussian ensemble is **universal**
- Other ensembles possible
  - $g(u) = \gamma |u|$, $g(u) = \gamma u^4$, ...

■ Nonconcave multifractals

Touchette & Beck, `cond-mat/0507379`, to appear in JSP





$$f \neq \tau^*$$

$$\tau = f^*$$

$$f = \tau_g^* + g$$

■ Other examples

- Thermodynamic formalism
  - Nonconvex spectra of dynamical indices:

$$P(\lambda) \sim e^{-t\psi(\lambda)}$$

- Fluctuation theorems
  - Nonconvex fluctuation functions:

$$P(W_t/t = w) \sim e^{-tf(w)}$$

- Large deviation theory
  - Nonconvex rate functions:

$$P(A_n = a) \sim e^{-nf(a)}$$

References

- M. Costeniuc, R.S. Ellis, H. Touchette, `cond-mat/0605213`, to appear in PRE
- H. Touchette, C. Beck, `cond-mat/0507379`, to appear in JSP
- M. Costeniuc, R.S. Ellis, H. Touchette, B. Turkington, *J. Stat. Phys.* **119**, 1283-1329, 2005.
- M. Costeniuc, R.S. Ellis, H. Touchette, B. Turkington, *Phys. Rev. E* **73**, 026105, 2006.

Work in collaboration with
Richard S. Ellis (UMass, USA)
Marius Costeniuc (Max Planck Inst., Germany)

Everything is extensive!

- Energy:

$$U \sim n, \qquad u = \frac{U}{n}$$

- Entropy:

$$\ln |\Omega_u| \sim n$$

$$s(u) = \lim_{n \to \infty} \frac{1}{n} \ln |\Omega_u|$$

- Free energy:

$$\ln Z(\beta) \sim n$$

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