Nonconcave entropies from generalized canonical ensembles

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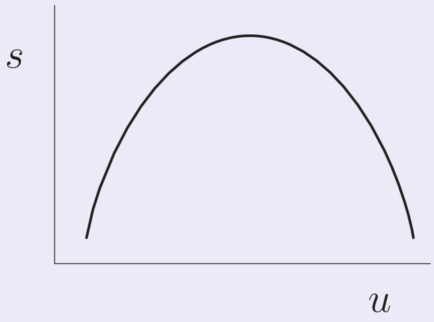
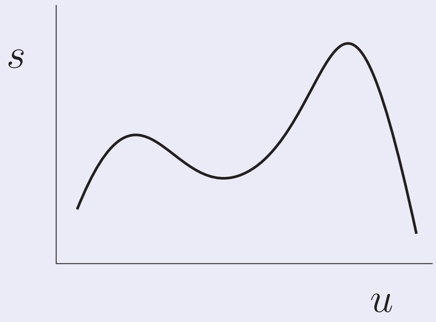
Outline

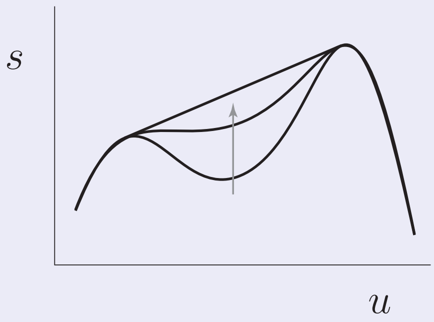
Short-range interactions



Long-range interactions



Small (finite) systems

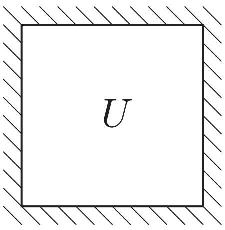


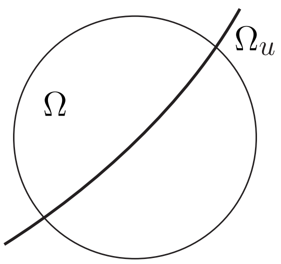
- Legendre transforms
- Equivalence of ensembles
- First-order phase transitions
- Metastable states

Plan

1. Review of concepts
2. Theory of nonconcave entropies
3. Generalized canonical ensembles
4. Applications

Microcanonical ensemble





Ω	Microstate space
$u = U/N$	Mean energy
Ω_u	Energy manifold

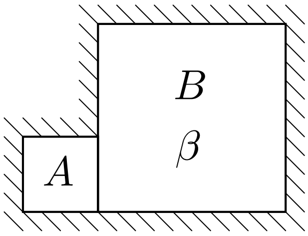
- Density of states:

$$\rho(u) = \# \text{ microstates in } \Omega_u = \text{volume}(\Omega_u)$$

- Entropy:

$$s(u) = \lim_{N\to\infty} \frac{1}{N} \ln \rho(u)$$

Canonical ensemble



$A \ll B$

$$\beta = \frac{1}{k_B T} = const, \qquad P = \frac{e^{-\beta U}}{Z(\beta)}$$

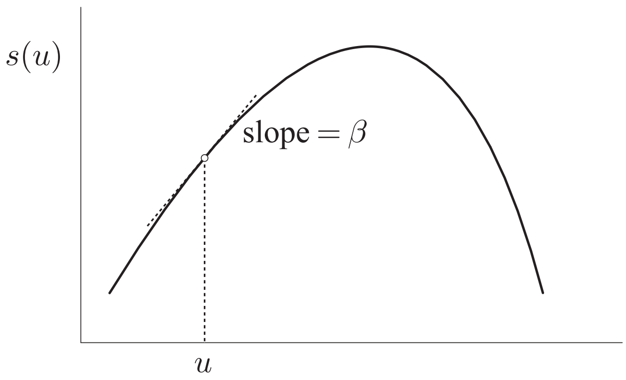
- Partition function:

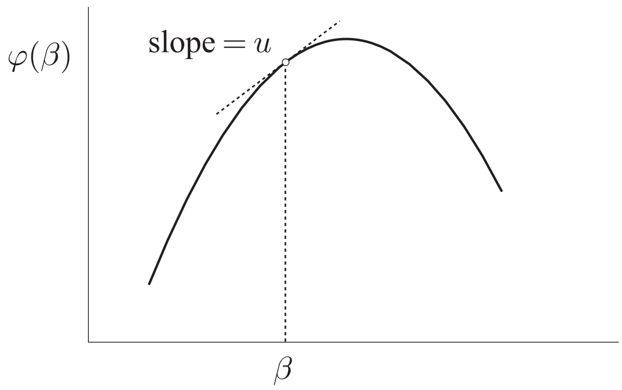
$$Z(\beta) = \sum_{\text{microstates}} e^{-\beta U}$$

- Free energy:

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

Legendre transform





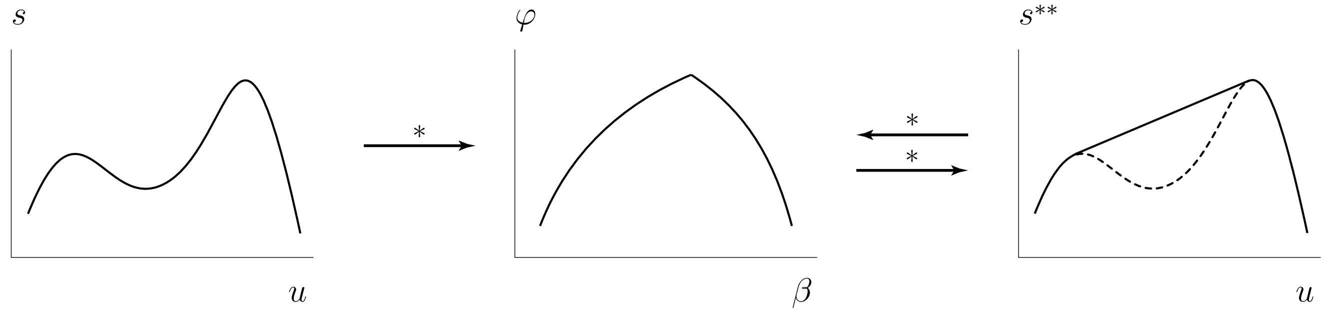
$$s(u) = \beta u - \varphi(\beta) \qquad \varphi(\beta) = \beta u - s(u)$$

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

$$s \longleftrightarrow \varphi$$
$$u \longleftrightarrow \beta$$

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

Nonconcave entropies



Non-concave
s

Always concave

$\varphi = s^*$

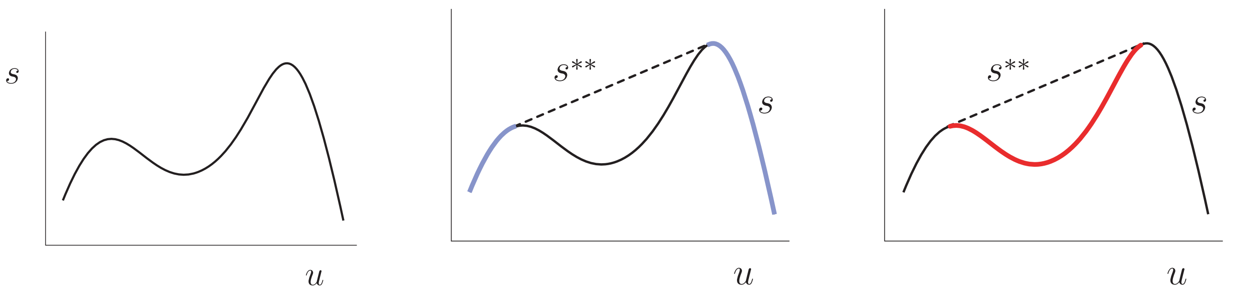
$s \neq s^{**}$

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

- $s^{**}(u)$ = concave envelope of $s(u)$
- $s^{**}(u) \geq s(u)$
- Nonequivalent ensembles
- Related to first-order phase transitions

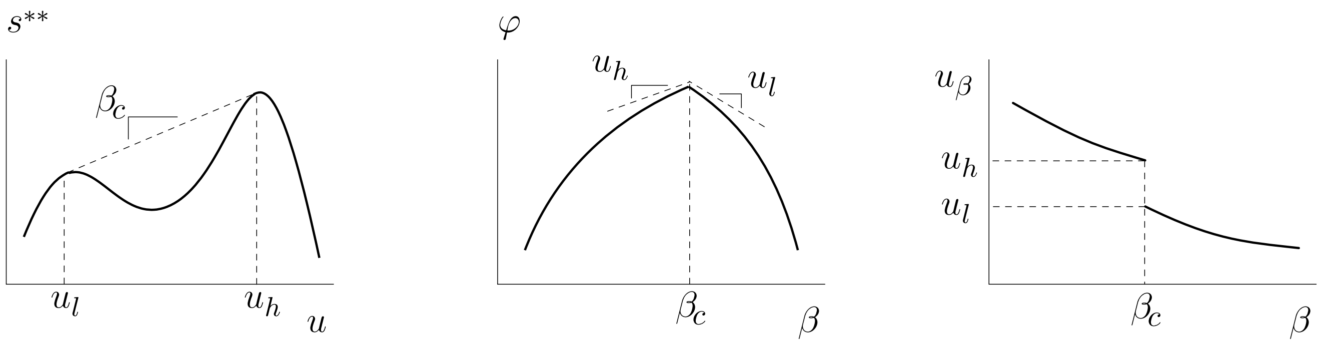
Nonequivalent ensembles

Eyink & Spohn 1993; Ellis, Haven & Turkington 2000



Thermodynamic level	$s = \varphi^*$	$s \neq \varphi^*$
Macrostate level	ME = CE	ME ≠ CE

First-order phase transitions



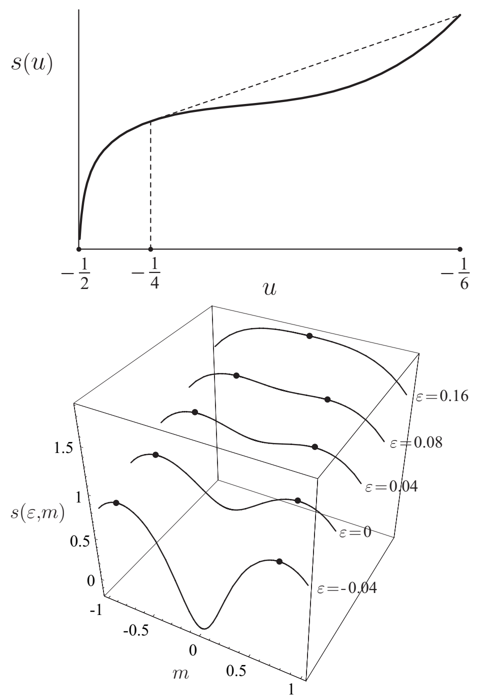
- $s(u)$ nonconcave $\Rightarrow$ $\varphi(\beta)$ non-differentiable
- First-order phase transition in canonical ensemble
- Latent heat: $\Delta u = u_h - u_l$

Canonical **skips** over microcanonical

Systems with nonconcave entropies

$$s \neq \varphi^*$$

- Gravitational systems
  - Lynden-Bell, Wood, Thirring (1960-)
  - Chavanis (2000-)
- Spin systems
  - Blume-Emery-Griffiths model
  - Mean-field Potts model ($q \geq 3$)
  - Mean-field ϕ^4 model
- 2D turbulence model
  - Point-vortex models, Onsagers
  - Kiessling & Lebowitz (1997)
  - Ellis, Haven & Turkington (2002)
- Multifractals



Long-range interactions

Generalized canonical ensembles

Costeniuc, Ellis, Touchette & Turkington, JSP 2005; PRE 2006

- N-particle system
- Energy: U
- Mean energy: $u = U/N$

Canonical

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

$$Z(\beta) = \sum_\omega e^{-N\beta u}$$

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

Generalized canonical

$$P_{g,\alpha} = \frac{e^{-N\alpha u - Ng(u)}}{Z_g(\alpha)}$$

$$Z_g(\alpha) = \sum_\omega e^{-N\alpha u - Ng(u)}$$

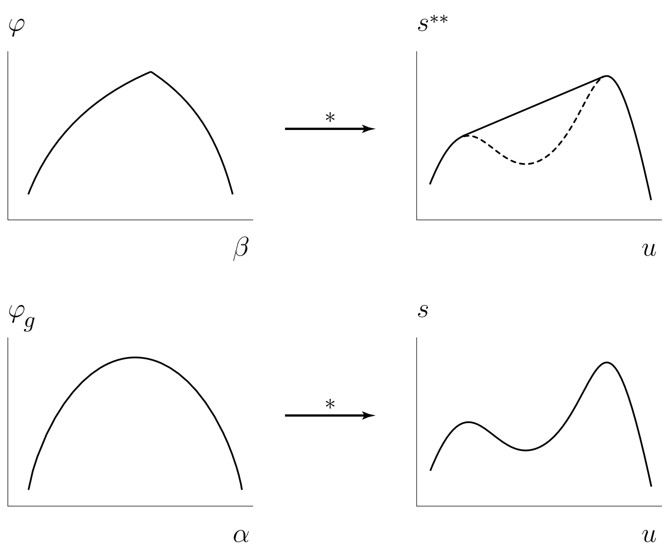
$$\varphi_g(\alpha) = \lim_{N\to\infty} -\frac{1}{N} \ln Z_g(\alpha)$$

Equivalence recovered

1. Choose g
2. Calculate $\varphi_g(\alpha)$

If $\varphi_g(\alpha)$ is differentiable at α, then

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



Exemple 1: Mean-field Potts model

Costeniuc, Ellis & Touchette PRE 2006

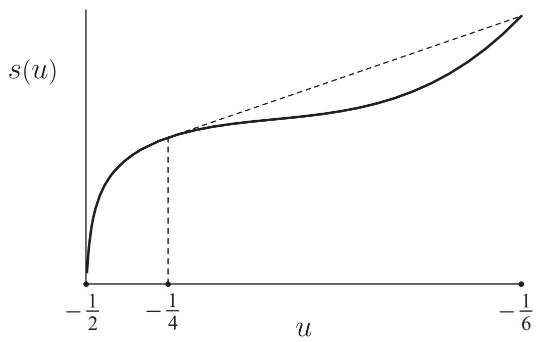
- Hamiltonian:

$$U(\omega) = -\frac{1}{2n}\sum_{i,k=1}^{n}\delta(\omega_i,\omega_k), \quad \omega_i \in \{1,2,3\}$$

- Mean energy:

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

- Entropy:



Costeniuc, Ellis & Touchette, JMP 2005

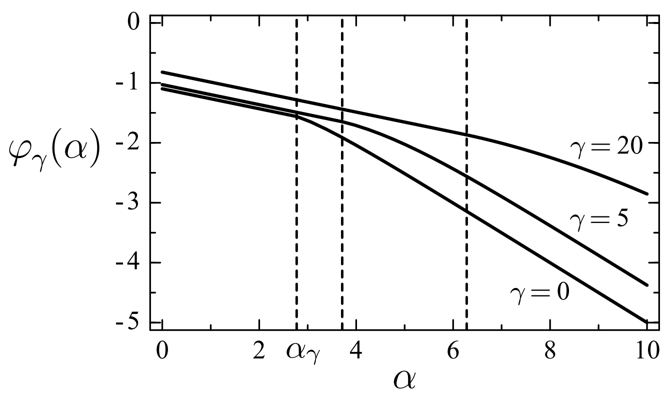
Gaussian ensemble

- Partition function:

$$Z_\gamma(\alpha) = \sum_{\text{microstates}} e^{-n\alpha u - n\gamma u^2}, \quad \alpha\in\mathbb{R}, \gamma>0$$

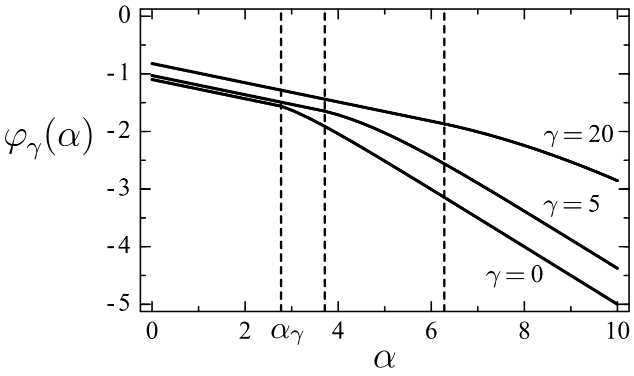
- Free energy:

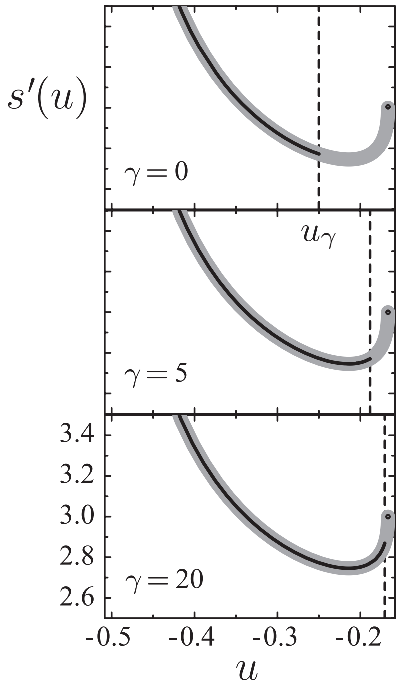
$$\varphi_\gamma(\alpha) = -\lim_{n\to\infty}\frac{1}{n}\log Z_\gamma(\alpha)$$



- Critical point: α_γ
- Branch 1: $\varphi'_\gamma(\alpha) = -\frac{1}{6}$
- Branch 2: $\varphi'_\gamma(\alpha) \in (-\frac{1}{2}, u_\gamma)$

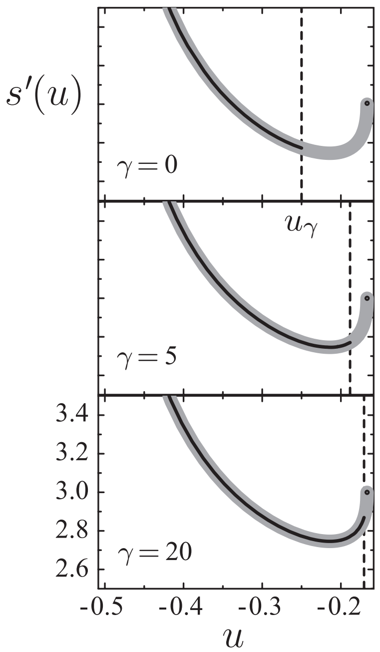
Calculation of the entropy

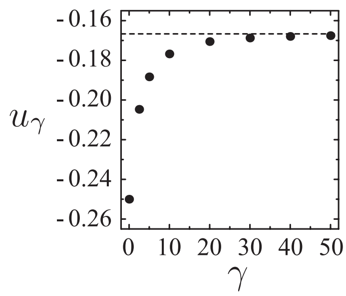


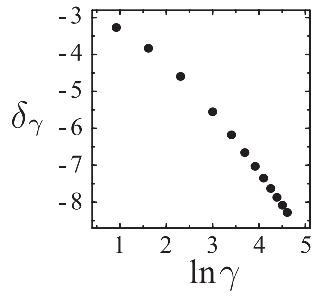


- Generalized Legendre transform
  - $s(u) = \alpha u + \gamma u^2 - \varphi_\gamma(\alpha)$
  - $u = \varphi'_\gamma(\alpha) \in (-1/2, u_\gamma)$

Asymptotic equivalence







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

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

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

Example 2: Two-block model

Touchette, Am. J. Phys. 2007

$$\boxed{\uparrow}\quad \boxed{\downarrow}\quad \cdots \quad \boxed{\uparrow}\qquad \boxed{\uparrow\quad \uparrow\quad \dots\quad \uparrow}\qquad \uparrow H$$

N free spins

$$U_1 = \sum_{i=1}^{N} s_i$$

$$s_i = \pm 1, \quad \mu H = 1$$

N frozen spins

$$U_2 = \sum_{i=1}^{N} s_i = N s_i$$

$$s_i = \pm 1$$

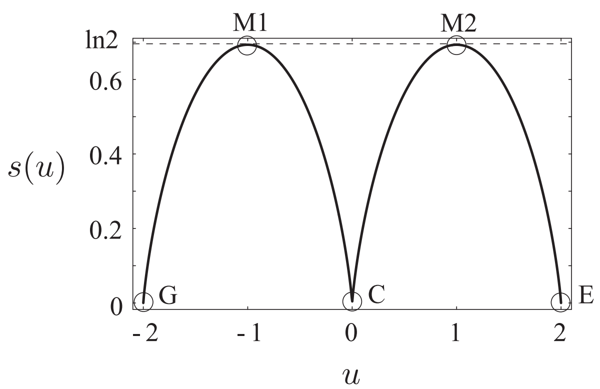
- Total energy:

$$U = U_1 + U_2$$

- Energy per spin:

$$u = \frac{U}{N} \in [-2, 2]$$

Entropy of the model



G : $\downarrow\downarrow\cdots\downarrow \mid \downarrow\downarrow\cdots\downarrow$

M1 : $\downarrow\uparrow\cdots\downarrow \mid \downarrow\downarrow\cdots\downarrow$

M2 : $\downarrow\uparrow\cdots\downarrow \mid \uparrow\uparrow\cdots\uparrow$

C : $\uparrow\uparrow\cdots\uparrow \mid \downarrow\downarrow\cdots\downarrow$

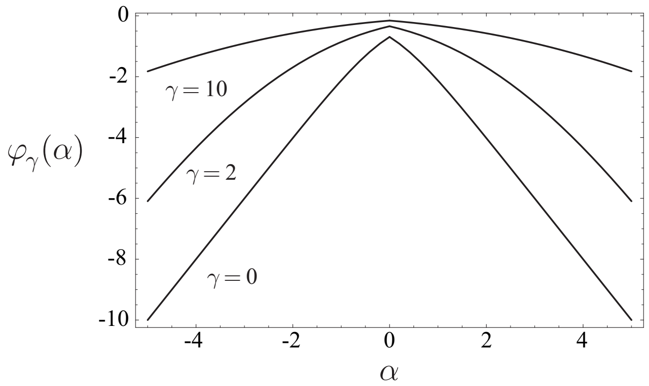
$\quad\ \ \downarrow\downarrow\cdots\downarrow \mid \uparrow\uparrow\cdots\uparrow$

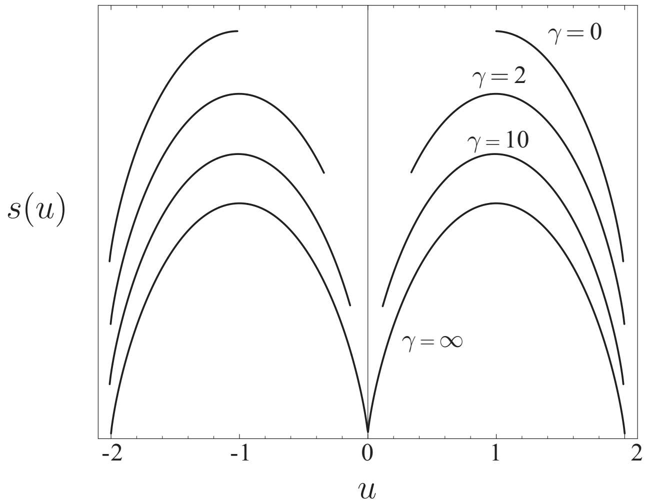
E : $\uparrow\uparrow\cdots\uparrow \mid \uparrow\uparrow\cdots\uparrow$

$$s(u) = \begin{cases} s_0(u+1) & u \in [-2, 0] \\ s_0(u-1) & u \in (0, 2] \end{cases}$$

$$s_0(u) = -\left(\frac{1-u}{2}\right) \ln\left(\frac{1-u}{2}\right) - \left(\frac{1+u}{2}\right) \ln\left(\frac{1+u}{2}\right)$$

Gaussian calculation of the entropy



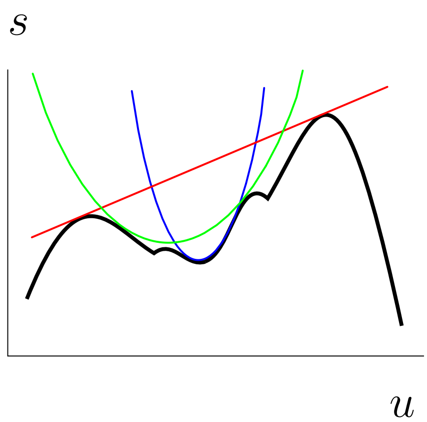


- Generalized Legendre transform:
  - $s(u) = \alpha u - \varphi_\gamma(\alpha) + \gamma u^2$
  - $\varphi'_\gamma(\alpha) = u$
- Asymptotic equivalence : $\gamma \to \infty$

Other ensembles?

$$Z_g(\alpha) = \sum_{\text{micro-états}} e^{-N\alpha u - Ng(u)}$$

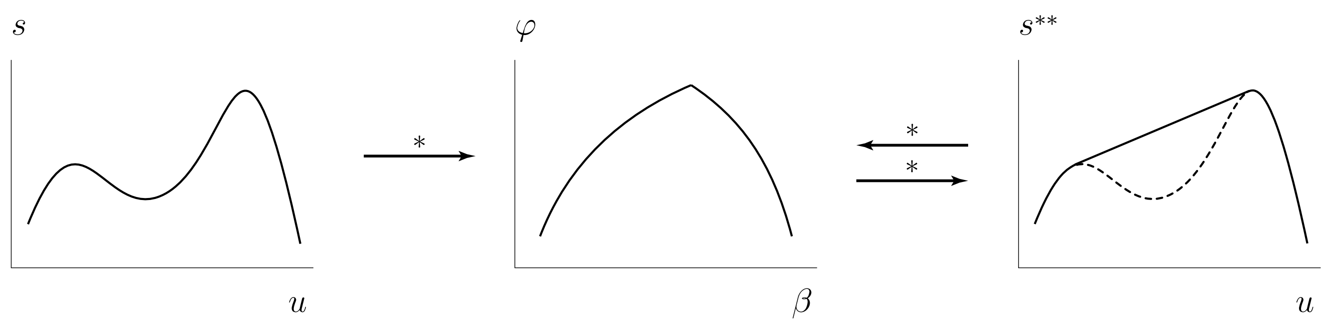
- Canonical:
  - $g = 0$
  - $g = \text{const}$
  - $g = \gamma u$
- Gaussian: $g(u) = \gamma u^2$
- Betrag: $g(u) = \gamma|u|$
- Others?



Universal equivalence

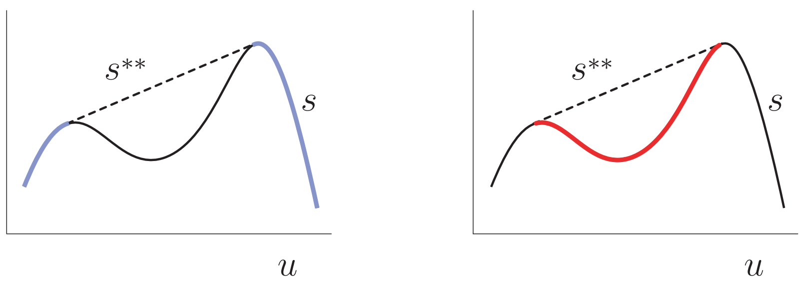
Any entropy function can be obtained via the Gaussian ensemble (possibly in the limit $\gamma \to \infty$)

Summary



- $s(u)$ can be nonconcave
- Ensemble nonequivalence: $s \neq \varphi^*$
- Related to first-order phase transitions
- Generalized canonical ensemble: $\varphi \to \varphi_g$
- Equivalence recovered: $s = \varphi_g^* + g$
- Gaussian ensemble is universal

Work in progress



- Metastable states
  - Metastability ⇔ nonconcave entropy
  - Equilibrium in ME = metastable or unstable in CE
  - Metastable in CE = equilibrium in generalized CE
- Multicanonical sampling

$$P(\omega) = ae^{-Nh(u(\omega))}$$

Some references

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