A simple spin model with a nonconcave entropy

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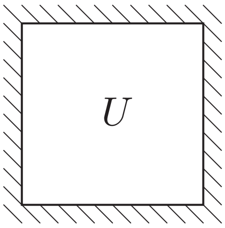
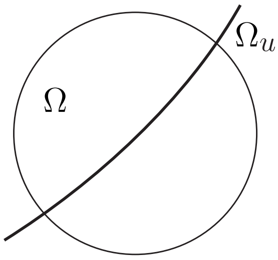
Outline

Microcanonical ensemble





Ω	microstate space
$u = U/N$	mean energy
Ω_u	energy shell
$P = const$	for microstate $\in \Omega_u$

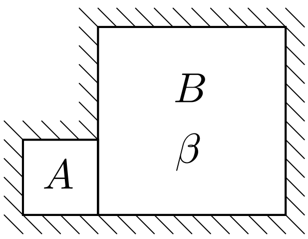
- Density of states:

$$\rho(u) = \#microstates\ with\ mean\ energy\ u$$

- Microcanonical entropy function:

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

Canonical ensemble



$A \ll B$

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

- Canonical partition function:

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

- Canonical free energy function:

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

Basic properties

Free energy

- $\varphi(\beta)$ is always concave
- $\varphi(\beta)$ is the Legendre transform of $s(u)$

$$\varphi(\beta) = \beta u_\beta - s(u_\beta), \qquad s'(u_\beta) = \beta$$

Entropy

- $s(u)$ is always concave
- $s(u)$ is the Legendre transform of $\varphi(\beta)$

$$s(u) = \beta_u u - \varphi(\beta_u), \qquad \varphi'(\beta_u) = u$$

Not always true!

- The microcanonical and canonical ensembles are always equivalent

Block spin model

Touchette, `cond-mat/0504020`

$$\boxed{\uparrow}\ \boxed{\downarrow}\ \cdots\ \boxed{\uparrow} \qquad \boxed{\uparrow\ \ \uparrow\ \ \ldots\ \ \uparrow} \qquad \uparrow H$$

N free spins

$$U_{free} = \sum_{i=1}^{N} s_i$$

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

N correlated (frozen) spins

$$U_{corr} = \sum_{i=1}^{N} s_i = N s_i$$

$$s_i = \pm 1$$

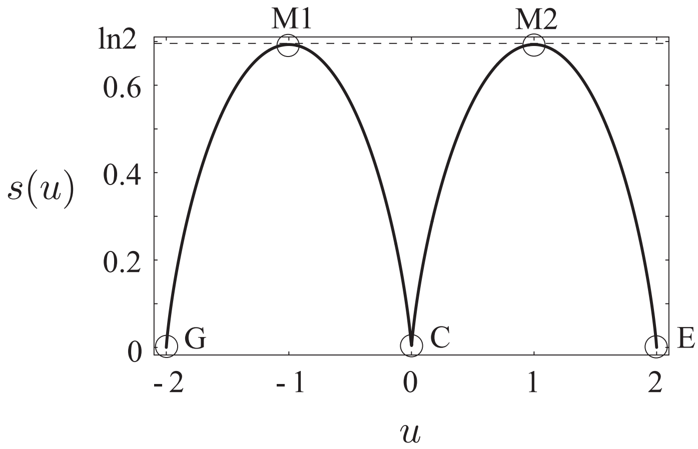
- Total energy:

$$U_{tot} = U_{free} + U_{corr}$$

- Mean energy:

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

Microcanonical entropy



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

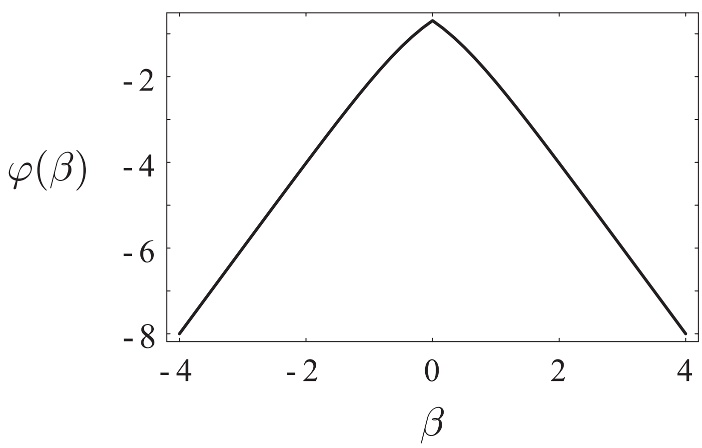
$\quad\;\; \downarrow\downarrow\cdots\downarrow \mid \uparrow\uparrow\cdots\uparrow$

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

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

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

Canonical free energy

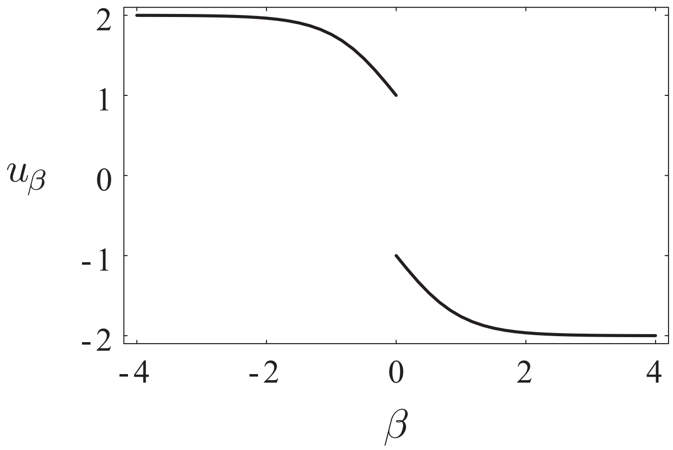


- Solution:

$$\varphi(\beta) = -\ln(2\cosh\beta) - |\beta|$$

- Non-differentiable at $\beta = 0$
- First-order phase transition in canonical ensemble

Equilibrium mean energy in canonical ensemble



$$u_\beta = \varphi'(\beta)$$

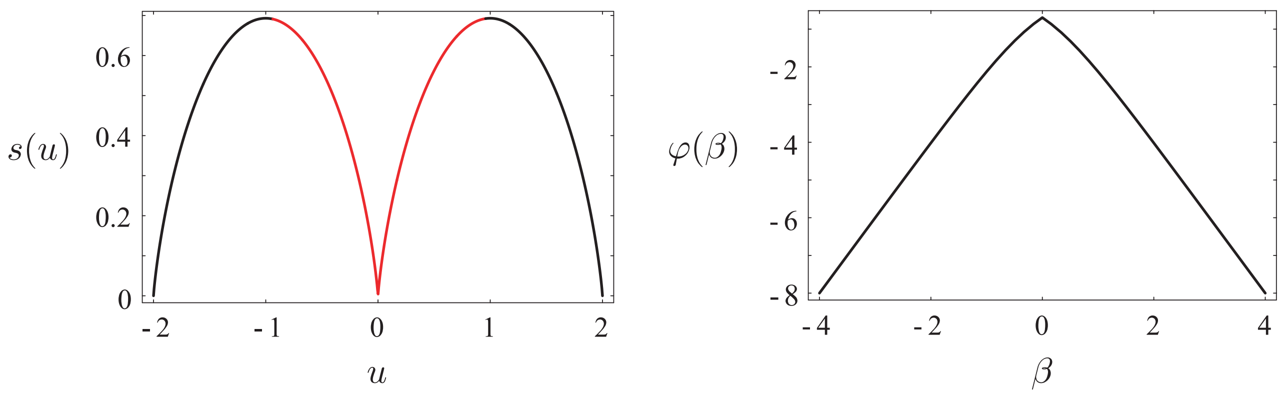
$\downarrow\uparrow \cdots \downarrow \mid \uparrow\uparrow \cdots \uparrow \quad u = +1$

$\downarrow$

$\downarrow\uparrow \cdots \downarrow \mid \downarrow\downarrow \cdots \downarrow \quad u = -1$

- First-order phase transition at $\beta = 0$
- Canonical "does not see" the mean energy region $u \in (-1, 1)$
- Nonequivalence of ensembles for $u \in (-1, 1)$

Nonequivalence of ensembles



- $\varphi = s^*$ always
- $s = \varphi^*$ for $u \notin (-1, 1)$
- $s \neq \varphi^*$ for $u \in (-1, 1)$

Generalized canonical ensemble

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

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

Standard canonical

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

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

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

Generalized canonical

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

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

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

Gaussian ensemble

Challa & Hetherington (1988)

- Pivot function: $g(u) = \gamma u^2$
- Gaussian Gibbs measure:

$$P_{\gamma,\alpha} = \frac{e^{-N\alpha u - N\gamma u^2}}{Z_\gamma(\alpha)}$$

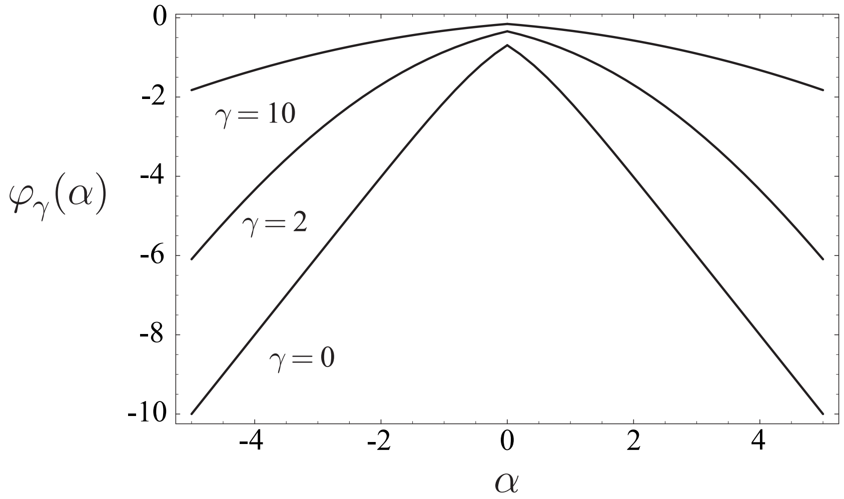
- Gaussian partition function:

$$Z_\gamma(\alpha) = \sum_{\textit{microstates}} e^{-N\alpha u - N\gamma u^2}$$

- Gaussian free energy:

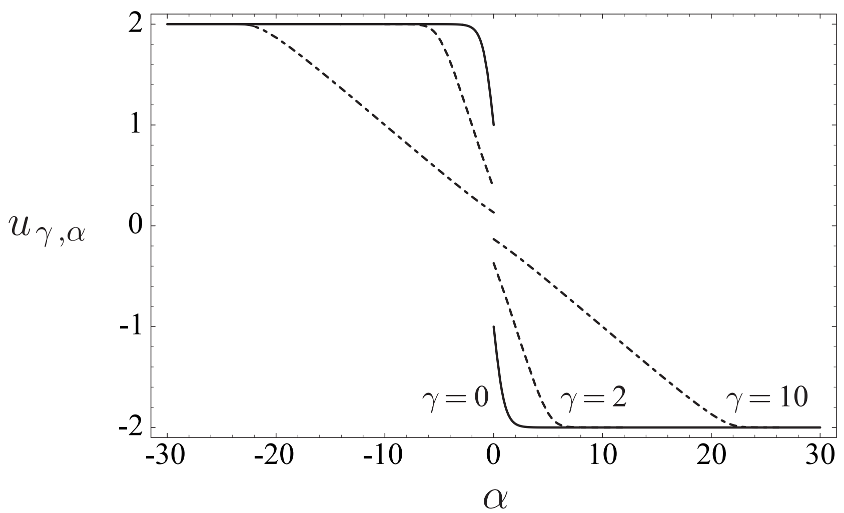
$$\varphi_\gamma(\alpha) = \lim_{N\to\infty} -\frac{1}{N} \ln Z_\gamma(\alpha)$$

Gaussian free energy



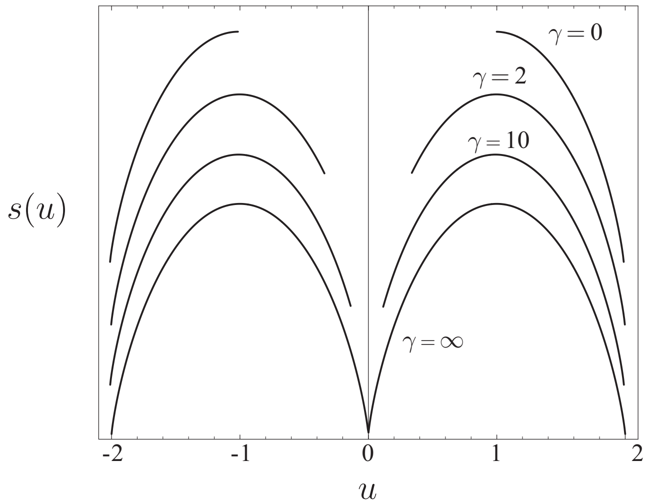
- Nondifferentiable point disappears as $\gamma \to \infty$
- Closing of the mean energy gap

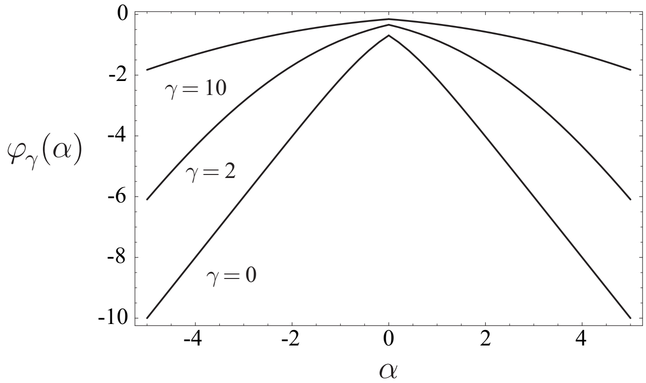
Equilibrium mean energy



- Equilibrium mean energy: $u_{\gamma,\alpha} = \varphi'_\gamma(\alpha)$
- Closing of the mean energy gap
- First-order phase transition disappears as $\gamma \to \infty$

Recovering the entropy



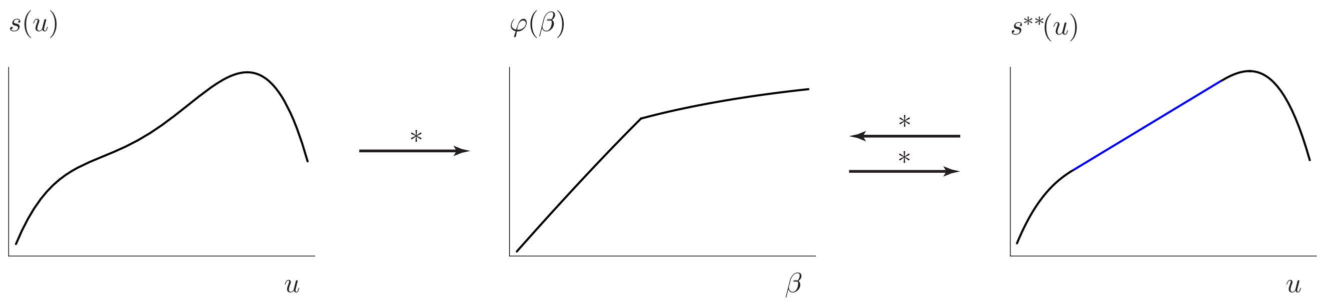


- Calculation of the entropy:

$$s(u) = \underbrace{\alpha_u u - \varphi_\gamma(\alpha_u)}_{\text{Legendre transform: } \varphi_\gamma^*} + \gamma u^2, \qquad \varphi_\gamma'(\alpha_u) = u$$

- Correct entropy recovered as $\gamma \to \infty$

Conclusion



- s is not necessarily concave
- If s is nonconcave, then $s \neq \varphi^*$
- Basis for nonequivalence of ensembles
- Related to first-order phase transitions
- Generalized canonical free energy: $\varphi \to \varphi_g$
- Recovering equivalence: $s = \varphi_g^* + g$

Systems with nonconcave entropies

- Gravitating particles (Thirring, Lynden-Bell, 1970s)
- Mean-field and long-range spin models
  - Blume-Emery-Griffiths model
  - Potts model ($q > 2$)
  - Hamiltonian mean-field model (ϕ^4)
- Model of plasma
- Statistical models of turbulence
- Typically: systems with long-range potentials

Other applications

Multifractals

Nonconcave multifractal spectrum:

$$n_\varepsilon(\alpha) \sim \varepsilon^{-f(\alpha)}$$

Touchette & Beck JSP (2006)

Nonequilibrium fluctuation theorems

Nonconvex fluctuation functions:

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

Large deviation theory

Nonconvex rate functions:

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

General references

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