Equilibrium systems with nonequivalent ensembles

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Outline

Equilibrium ensembles

- N-particle system
- Hamiltonian: $H(\omega)$
- Macrostate: $M(\omega)$

Microcanonical $u = H/N$ ME

$$P^u(\omega) = \text{const} \cdot \delta_{\Lambda|u}$$

- Density of states:

$$\Omega(u) = \int \delta(H(\omega) - uN)\, d\omega$$

- Entropy:

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

- Equilibrium states:

$$\mathcal{E}^u = \{m^u\}$$

Canonical β CE

$$P_\beta(\omega) = e^{-\beta H(\omega)}/Z(\beta)$$

- Partition function:

$$Z(\beta) = \int e^{-\beta H(\omega)}\, d\omega$$

- Free energy:

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

- Equilibrium states:

$$\mathcal{E}_\beta = \{m_\beta\}$$

Equivalence of ensembles

$$\text{ME} \stackrel{?}{=} \text{CE}$$

Thermodynamic level

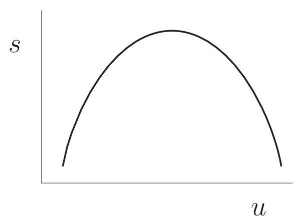
$$u \stackrel{?}{\longleftrightarrow} \beta$$
$$s(u) \stackrel{?}{\longleftrightarrow} \varphi(\beta)$$

Macrostate level

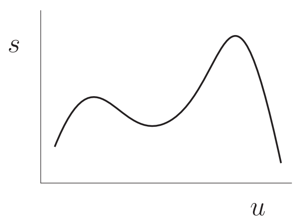
$$\mathcal{E}^u \stackrel{?}{\longleftrightarrow} \mathcal{E}_\beta$$

- Short-range systems have equivalent ensembles
- Long-range systems may have nonequivalent ensembles
- Related to concavity of $s(u)$

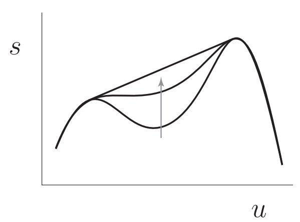
Short-range



Long-range



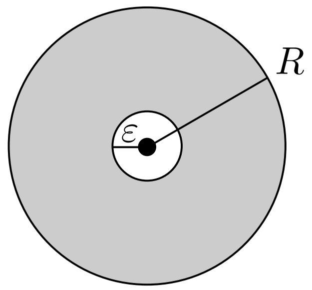
Small (finite)



Short- vs long-range interactions

- Potential:

$$V(r) = \frac{c}{r^\alpha}$$



- Interaction energy:

$$U = \int_\varepsilon^R V(r)\, d^d r \propto \begin{cases} R^{d-\alpha} & \alpha \neq d \\ \ln R & \alpha = d \end{cases}$$

Short-range interaction

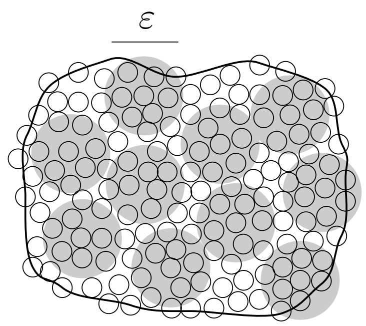
- $\alpha > d$

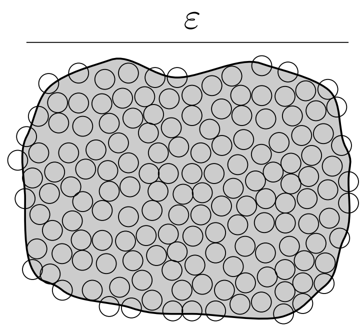
Long-range interaction

- $\alpha < d$

	α	α/d	Type
Collisions	∞	∞	short
Gravity	1	1/3	long
Coulomb	1	1/3	long (short)
Mean-field	0	0	long (∞)

Short- vs long-range interactions (cont'd)





- Finite-range interaction
- Finite correlation length
- Extensive energy: $U \sim N$
- Bulk dominates over surface
- Sub-system separation
- Entropy always concave

- Interaction is 'infinite' range
- Infinite correlation length
- Non-extensive energy
- Bulk $\sim$ surface
- No separation
- Entropy possibly nonconcave

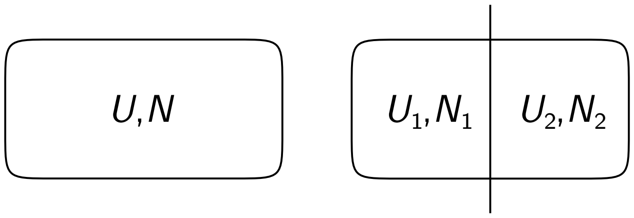
Concave entropy – Short-range

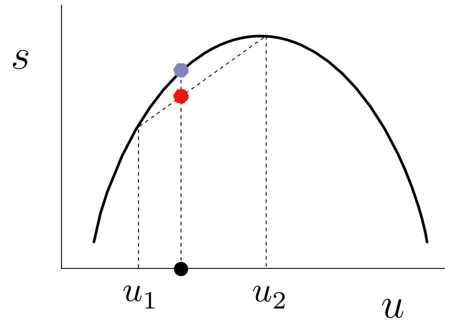
[Ruelle, Lanford 1960s]

- Entropy:

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

- Separation argument:





$$U \approx U_1 + U_2$$

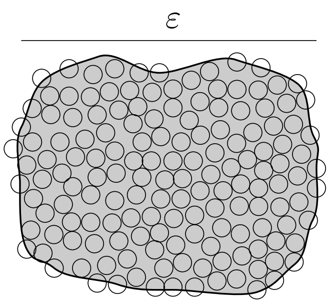
$$\Omega_N(U_1 + U_2) \geq \Omega_{N_1}(U_1)\, \Omega_{N_2}(U_2)$$

$$s(\alpha u_1 + \bar{\alpha} u_2) \geq \alpha s(u_1) + \bar{\alpha} s(u_2)$$

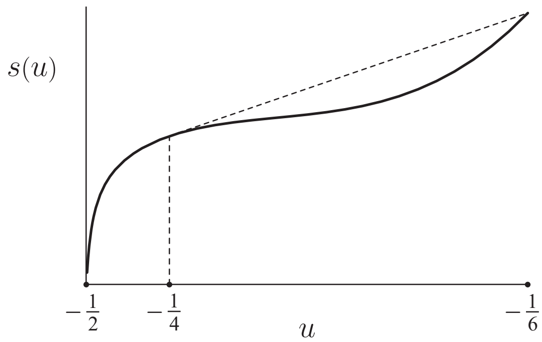
Nonconcave entropies – Long-range

[Lynden-Bell 1969, Thirring 1970, Gross 1997]

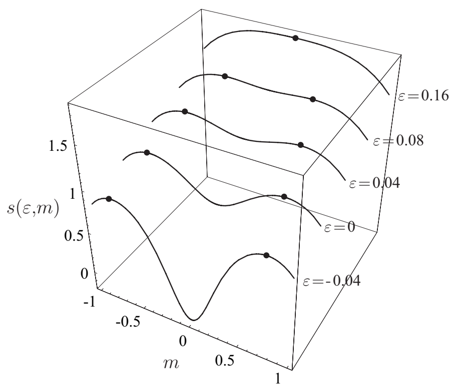
- Interaction is 'infinite' range
- No separation possible
- Entropy can be nonconcave



Mean-field Potts model

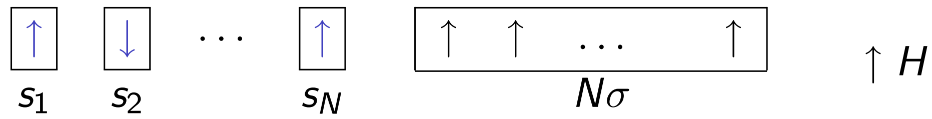


Mean-field ϕ^4 model



Two-block spin model

[HT Am J Phys 2008]

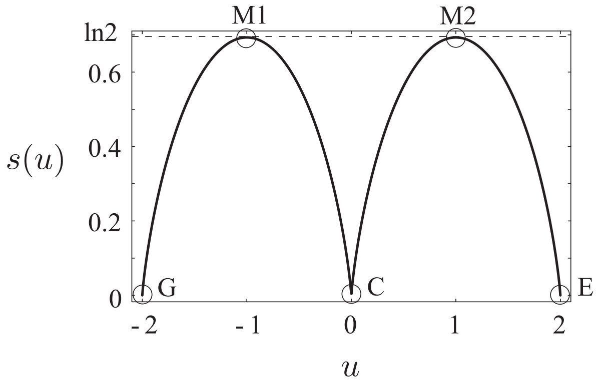


- Total energy: $U = \sum_{i=1}^{N} s_i + N\sigma$
- Energy per spin:

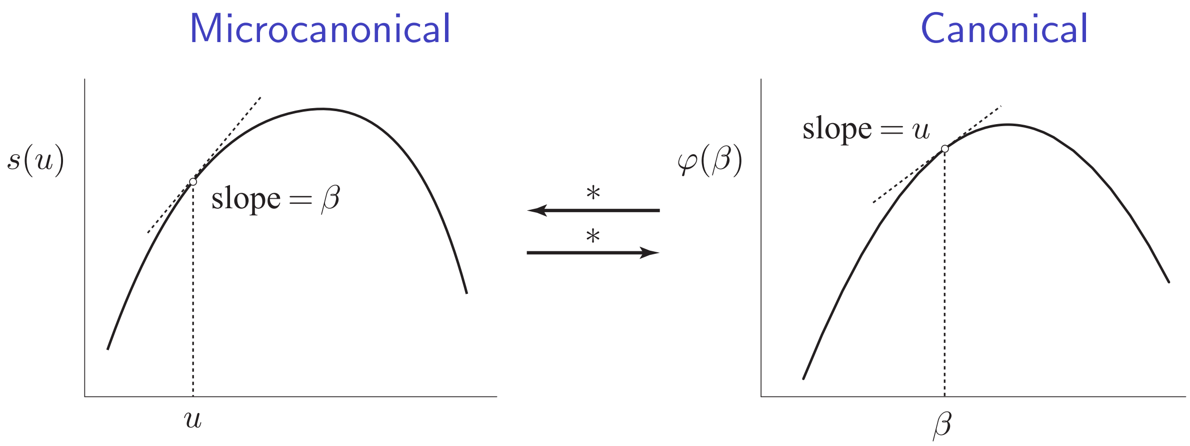
$$u = \frac{U}{N} \in [-2, 2]$$

- Entropy:

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



Legendre duality



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

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

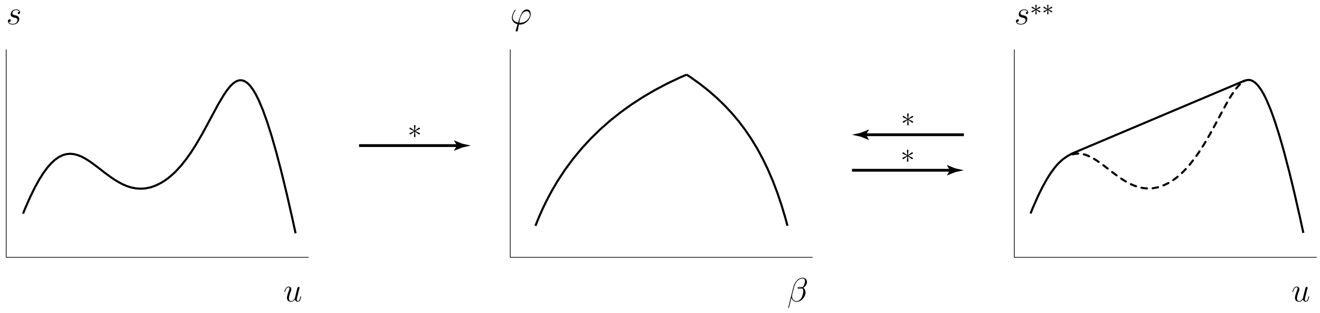
$$s \longleftrightarrow \varphi$$
$$u \longleftrightarrow \beta$$

$$s = \varphi^*$$

$$\varphi = s^*$$

Thermodynamic equivalence of ensembles

Breakdown of Legendre duality



Non-concave
s

Always concave

$\varphi = s^*$

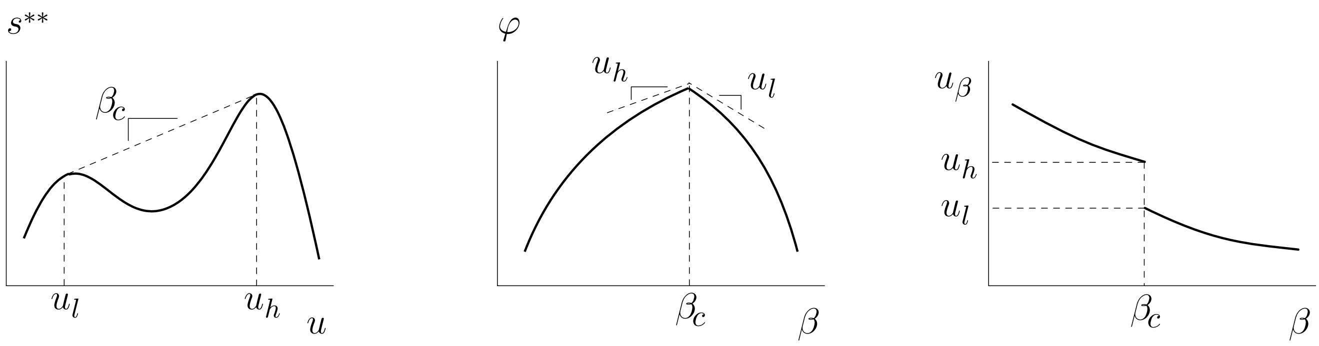
$s \neq s^{**}$

$s \neq \varphi^*$

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

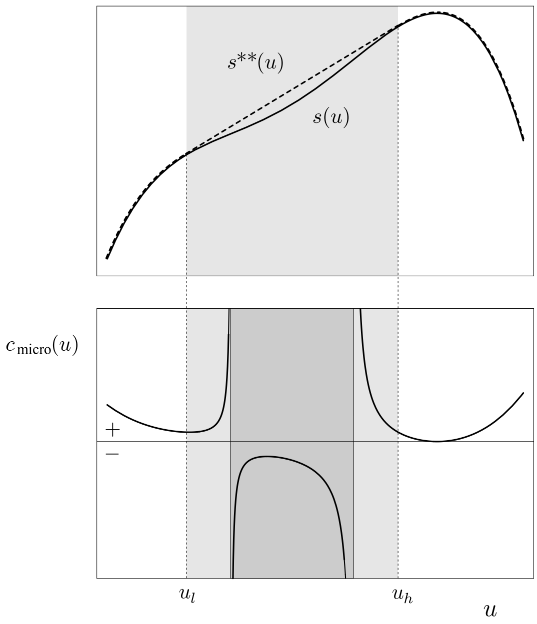
Thermodynamic nonequivalence of ensembles

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

Negative heat capacities



$$c = \frac{du}{dT}$$

Canonical

- $T = \beta^{-1}$
- $u = u_\beta$

$$c_{\text{can}}(\beta) = -\beta^2 \varphi''(\beta) > 0$$

Microcanonical

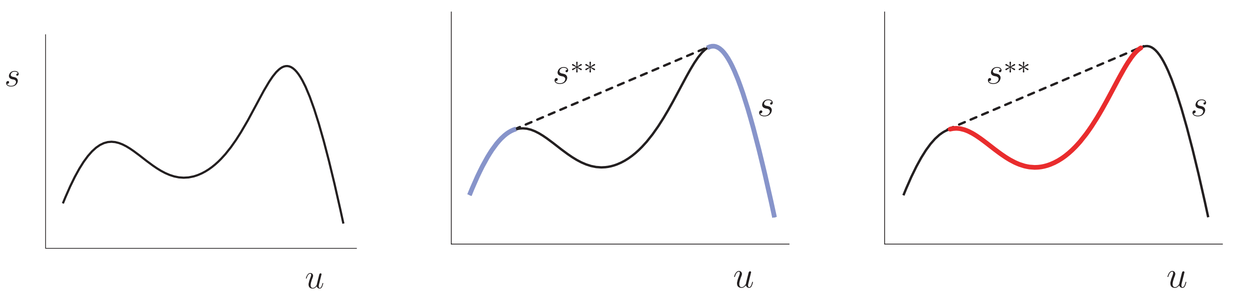
- u
- $T = s'(u)^{-1}$

$$c_{\text{micro}}(u) = -s'(u)^2\ s''(u)^{-1}$$

$c_{\text{micro}} < 0 \Rightarrow s$ is nonconcave

Macrostate nonequivalence

[Eyink & Spohn JSP 1993; Ellis, Haven & Turkington JSP 2000]

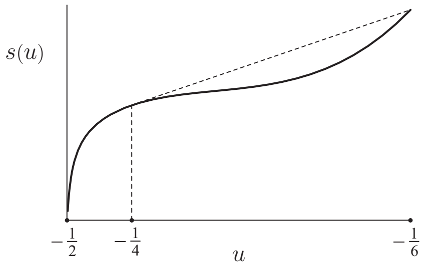


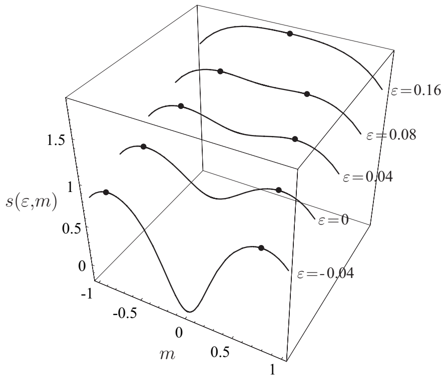
Thermo level	$s = \varphi^*$	$s \neq \varphi^*$
Macrostate level	$\mathcal{E}^u = \mathcal{E}_\beta$	$\mathcal{E}^u \neq \mathcal{E}_\beta$

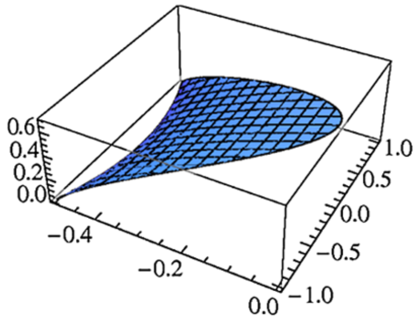
Systems with nonconcave entropies

[Campa, Dauxois & Ruffo Phys Rep 2009]

- Gravitational systems
  - Lynden-Bell, Wood, Thirring (1960-)
  - Chavanis (2000-)
- Spin systems
  - Mean-field Blume-Emery-Griffiths model
  - Mean-field Potts model ($q \geq 3$)
  - Mean-field ϕ^4 model
- 2D turbulence model
  - Point-vortex models (Onsager, 1949)
  - Kiessling & Lebowitz (1997)
  - Ellis, Haven & Turkington (2002)
- Optical lattices (quantum spins)
  - Kastner (2010)







Gravitational systems

[Lynden-Bell, Wood, Thirring (60s and 70s), Chavanis (2000)]

- Total energy:

$$E = \langle K \rangle + \langle V \rangle$$

- Virial theorem:

$$2\langle K \rangle + \langle V \rangle = 0$$

- Energy:

$$E = -\langle K \rangle < 0 \quad \text{bound state}$$

- Kinetic temperature:

$$T \propto \langle K \rangle$$

- Heat capacity:

$$C = \frac{dE}{dT} \propto \frac{dE}{d\langle K \rangle} < 0$$

  - $T \searrow$ when $E \nearrow$

Mean-field Potts model

[Ispolatov & Cohen Physica A 2000; Costeniuc, Ellis & HT JMP 2005]

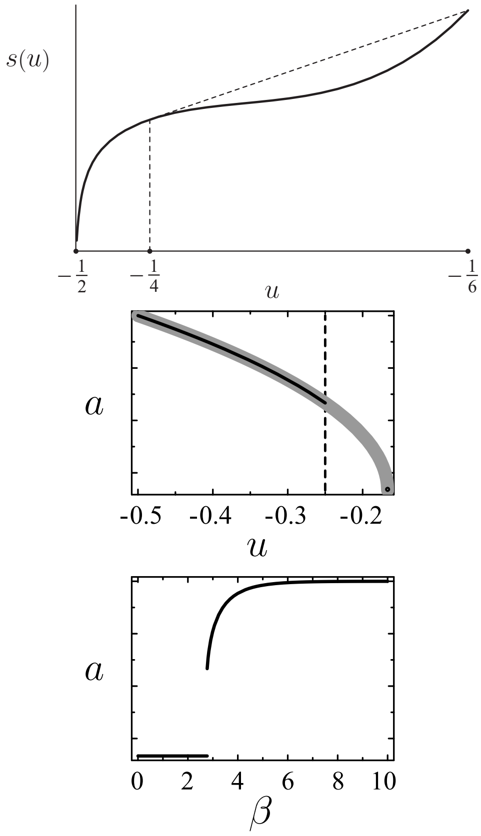
- Hamiltonian:

$$H = -\frac{1}{2N}\sum_{i,j=1}^{N} \delta_{\omega_i,\omega_j}, \quad \omega_i \in \{1,2,3\}$$

- Distribution of spins: $\nu = (a, b, b)$
- Macrostate:

$$a = \frac{\#\text{ spins } 1}{N}$$

  - ME macrostate: $a(u)$
  - CE macrostate: $a(\beta)$
- Nonconcave entropy
  - Nonequivalent ensembles
  - First-order canonical phase transition
  - Metastable states



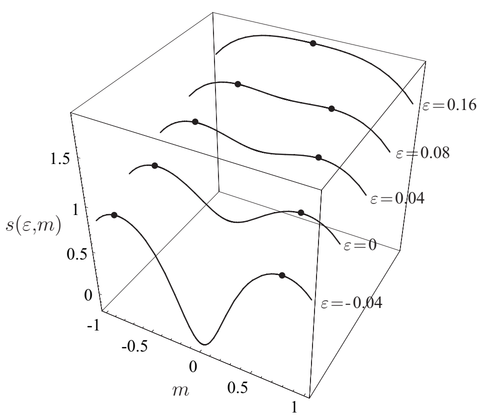
ϕ^4 model

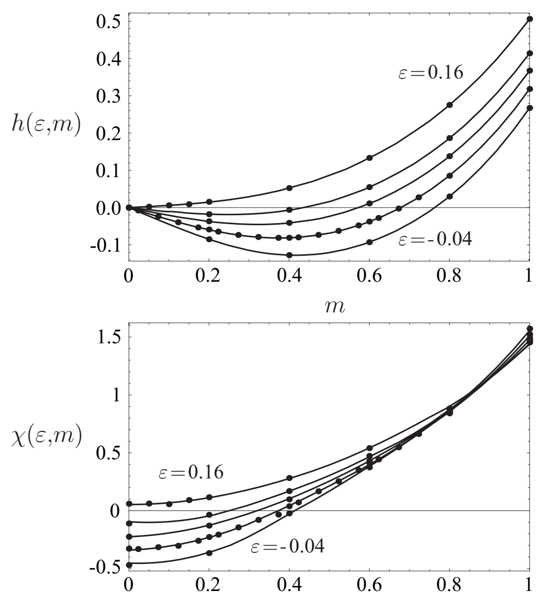
[Campa, Ruffo & HT, Physica A 2007]

- Hamiltonian:

$$H = \sum_{i=1}^{N}\left(\frac{p_i^2}{2} - \frac{q_i^2}{4} + \frac{q_i^4}{4}\right) - \frac{1}{4N}\sum_{i,j=1}^{N} q_i q_j, \quad p_i, q_i \in \mathbb{R}$$

- Magnetisation: $m = \frac{1}{N}\sum_{i=1}^{N} q_i$
- Entropy: $s(\varepsilon, m)$
- Effective field: $h = -T\partial_m s$
- Susceptibility: $\chi = (\partial_m h)^{-1}$

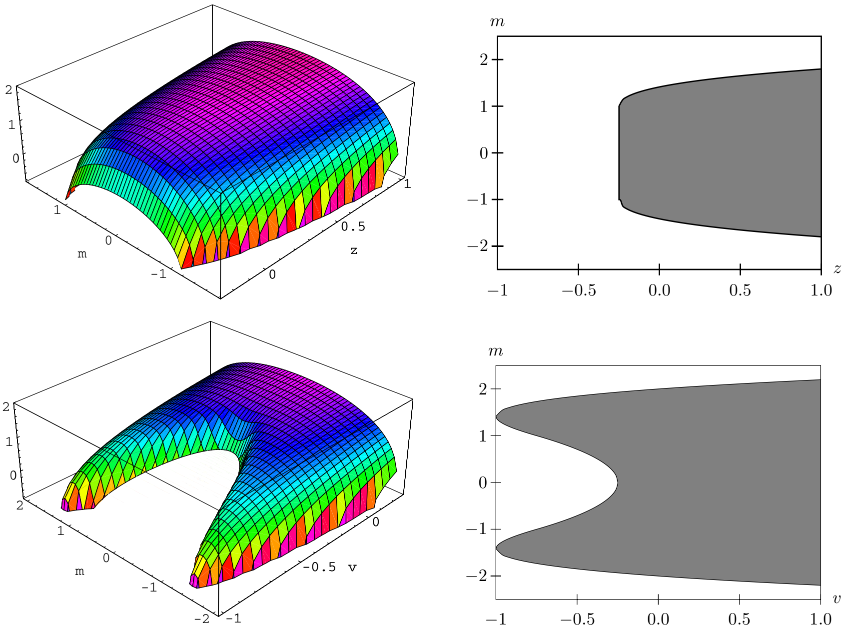




ϕ^4 variants

[Hahn & Kastner 2006]

$$H = \underbrace{\sum_{i=1}^{N} \left(\frac{q_i^4}{4} - \frac{q_i^2}{N} \right)}_{V} - \frac{J}{2N} \left(\sum_{i=1}^{2} q_i \right)^2$$



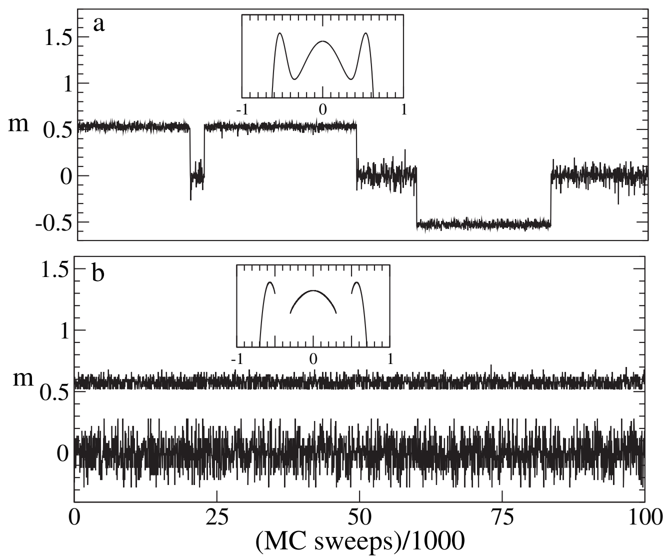
$J = 0$

$J \neq 0$

Recent research: Ergodicity breaking

[Mukamel et al PRL 2005, Bouchet et al PRE 2008]

- Nonconcave entropies can have disconnected support
- Disconnected macrostate regions
- Non-ergodic microcanonical dynamics



Generalized canonical ensemble

[Costeniuc, Ellis, HT & Turkington JSP 2005; Costeniuc, Ellis & HT PRE 2006]

Canonical ensemble

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

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

$$s \neq \varphi^*$$

Generalized canonical ensemble

$$Z_g(\beta) = \sum_{\omega} e^{-\beta U - Ng(U/N)}$$

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

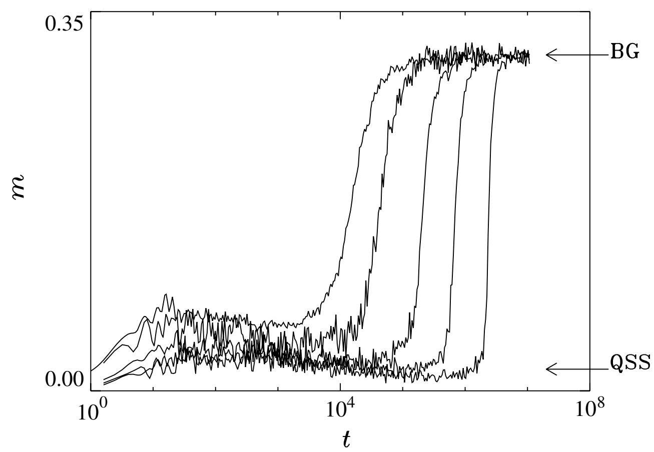
$$s = \varphi_g{}^* + g$$

- Recover equivalence with modified Legendre transform
- Gaussian ensemble: $g(u) = \gamma u^2$
- Betrag ensemble: $g(u) = \gamma|u - u_0|$
- Universal ensembles: equivalence recovered with $\gamma \to \infty$

Quasi-stationary states

[Campa, Dauxois & Ruffo Phys Rep 2009]

- Long-lived states $\neq$ ME or CE equilibrium states
- Nonequilibrium states
- First observed in Hamiltonian mean-field model
- Described using Vlasov equation (kinetic theory)
- Generic for long-range systems?

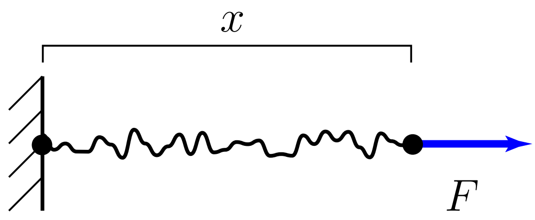


Other ensembles: DNA stretching experiments

[Cluzel et al Science 1996, Sinha & Samuel PRE 2005]

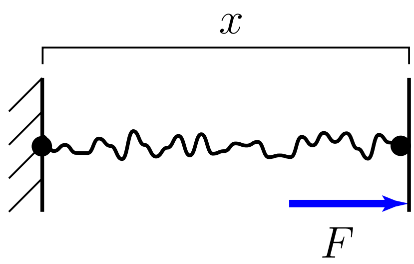
Isotensional ensemble

- Force: $F = \text{cte}$
- Extension: x fluctuates
- $\langle x \rangle$ vs F



Isometric ensemble

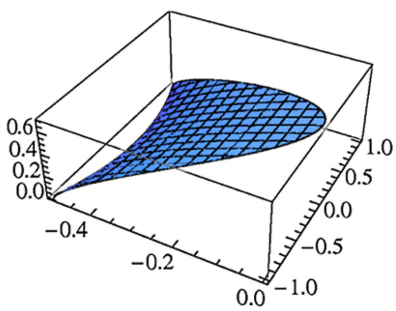
- Force: F fluctuates
- Extension: $x = \text{cte}$
- $\langle F \rangle$ vs x



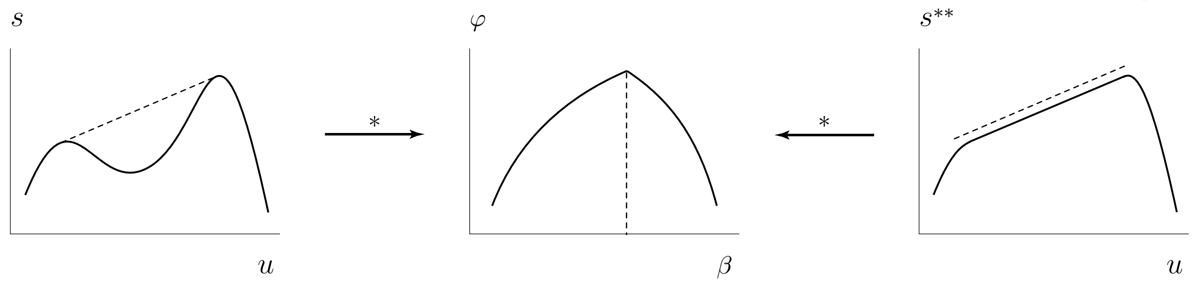
- Single molecule: Different ensembles
- Generally equivalent in thermo limit
- Possibly nonequivalent

Other topics

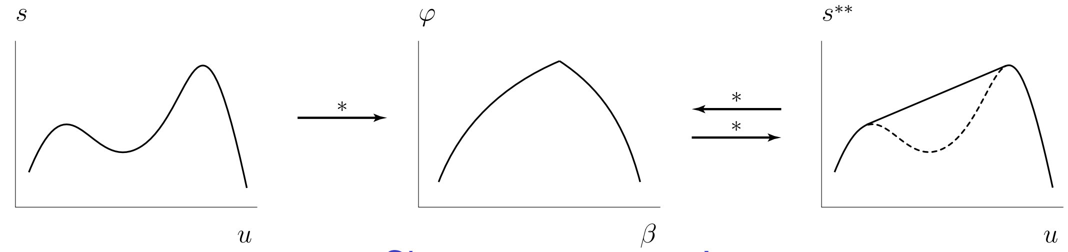
- 2D turbulence (point-vortex models with log interactions)
  [Kiessling & Lebowitz LMP 1997]
  [Turkington et al PNAS 2001; Ellis, Haven & Turkington 2002]
  [Venaille & Bouchet PRL 2009]
  - Application: Great Red Spot of Jupiter (ME = energy, circulation)
  - Geophysical flows
- Quantum systems [Kastner PRL 2010]
  - Noncommuting macrostates? e.g., E and M



- Nonconcave vs affine entropies
  [HT, Harris & Tailleur PRE 2010]



Conclusion



	Short-range	Long-range
Entropy	Always concave	Possibly nonconcave
Legendre transform	Duality	Possibly non-dual
Equivalent ensembles	Yes	Possibly nonequivalent
First-order PT	Affine $s(u)$	Affine/nonconcave $s(u)$

Open problems

- What type of interaction leads to nonequivalent ensembles?
- Experimental measurements of nonconcave entropies?

References

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