From nonconcave entropies to nonconvex fluctuation functions

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Many-body systems far from equilibrium:
Fluctuations, slow dynamics and long-range interactions

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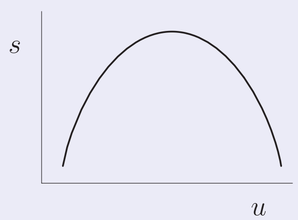
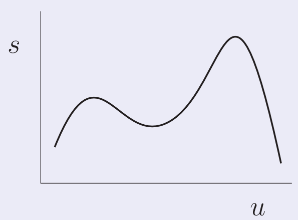
Outline

1. Long-range systems
2. Nonconcave entropies
3. Nonequilibrium fluctuations
4. Nonconvex rate functions

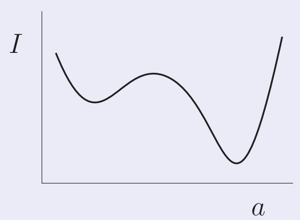
Concave



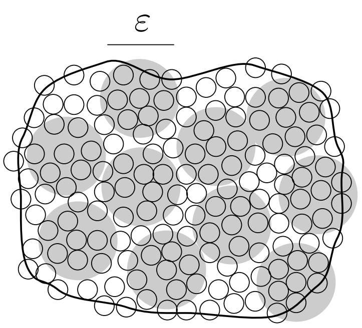
Nonconcave

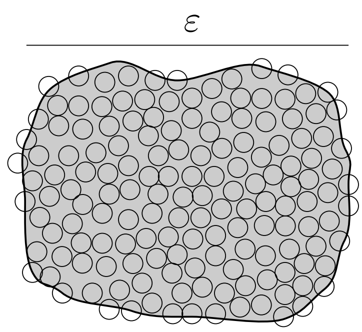


Nonconvex



From short- to long-range systems





- Short-range interaction
- Finite correlation length
- Extensive energy: $U \sim N$
- Sub-system separation

Entropy always concave

- Long-range interaction
- Infinite correlation length
- Non-extensive energy
- No separation

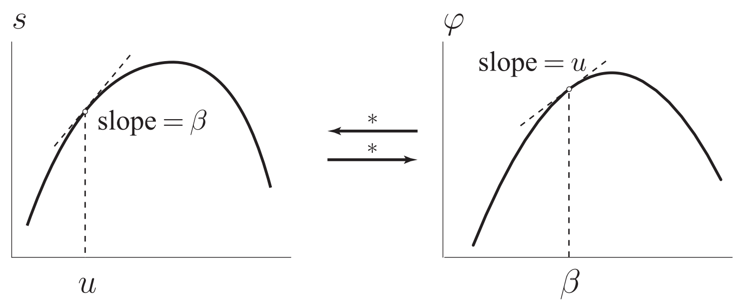
Entropy possibly nonconcave

Breakdown of the Legendre duality

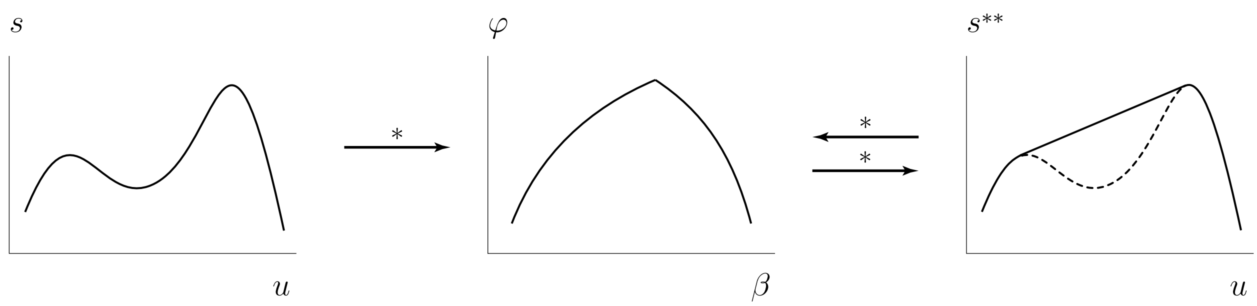
- Concave entropy:

$$\varphi = s^*$$

$$s = \varphi^*$$



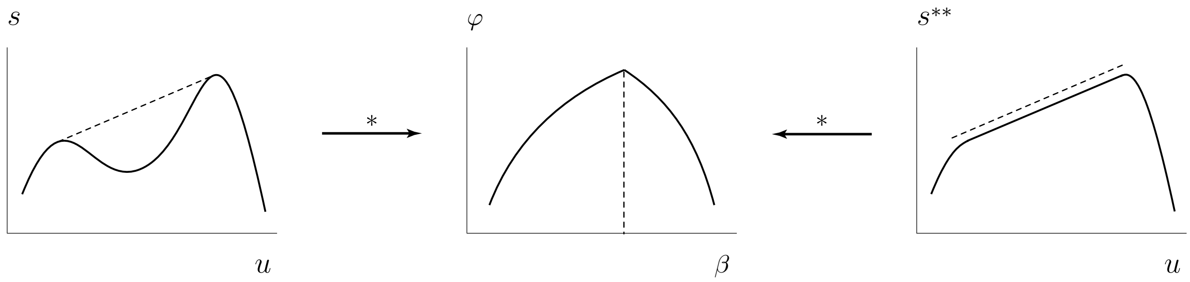
- Nonconcave entropy:



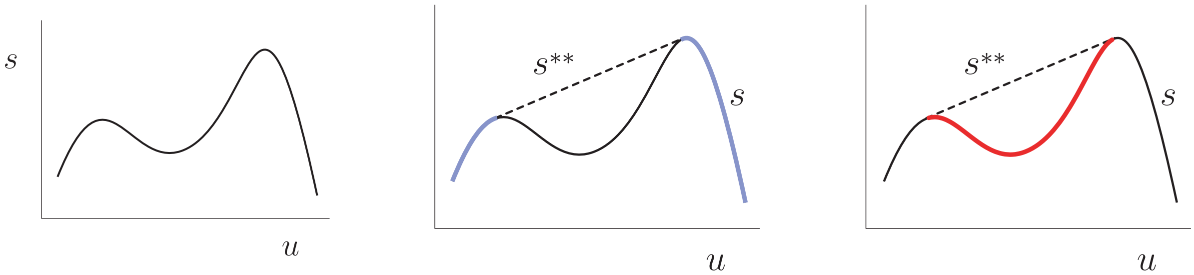
  - $s^{**}(u) =$ concave envelope of $s(u)$
  - $s^{**}(u) \geq s(u)$

Physical consequences

- Phase transitions



- Metastability



- Nonequivalent ensembles

How do we compute nonconcave entropies?

Large deviation formulation

- Random variable: A_n
- Probability distribution: $P(A_n = a)$

Large deviation principle

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

- Rate function: $I(a)$

- Generating function:

$$W_n(k) = \langle e^{nkA_n} \rangle$$

- Free energy:

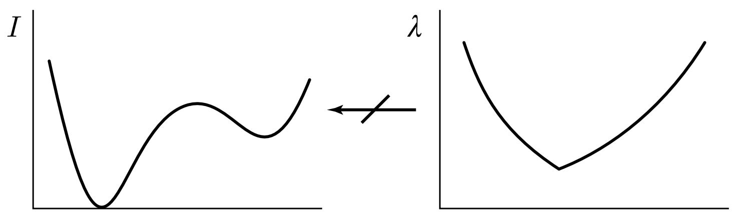
$$\lambda(k) = \lim_{n\to\infty} \frac{1}{n} \ln W_n(k)$$

Convex rate function

$$I = \lambda^*$$

Nonconvex rate function

$$I \neq \lambda^*$$



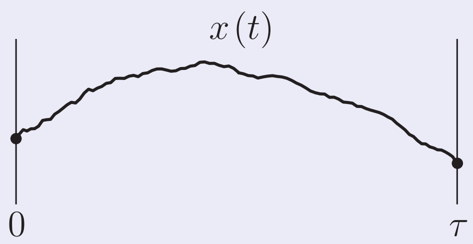
Entropies vs rate functions

Equilibrium entropy

- Microstate: $\omega = (\omega_1, \omega_2, \ldots, \omega_N)$
- Energy: $U(\omega)$
- Density of states: $\Omega_N(u)$
- Entropy: $\Omega_N(u) \sim e^{Ns(u)}$

Nonequilibrium fluctuations

- Trajectory: $x(t)$
- Process: $P[x]$
- Observable: $A_t[x]$
- Probability distribution: $P(A_t = a)$
- LDP: $P(A_t = a) \sim e^{-tI(a)}$



Problem

How to calculate nonconcave s or nonconvex I?

Method 1: Contraction

- Contraction: $A_n = f(B_n)$
- LDP for B_n: $P(B_n = b) \sim e^{-nI_B(b)}$

Contraction principle

LDP for A_n:

$$I_A(a) = \inf_{b:f(b)=a} I_B(b)$$

- Basis of MaxEnt principle / saddle-point approx
- Useful when $I_B(b)$ is convex
- Equilibrium applications:
  - BEG model (Barré et al PRL 2001; Ellis, Touchette & Turkington 2004)
  - HMF, $1/r^\alpha$ model (Barré et al JSP 2005)
  - Potts model (Costeniuc, Ellis & Touchette JMP 2005)
  - ϕ^4 model (Campa, Ruffo & Touchette 2008)

Method 2: Critical points of generating function

- Generating function:

$$W_n(k) = \langle e^{nkA_n} \rangle = \int e^{nL_k(\phi)}\, d\phi$$

- Free energy:

$$\lambda(k) = \sup_{\phi} L_k(\phi)$$

Critical point analysis

- Critical points of $L_k(\phi) \rightarrow I(a)$
- Global max of $L_k(\phi) \rightarrow$ convex parts of $I(a)$
- Local max and saddles of $L_k(\phi) \rightarrow$ nonconvex parts of $I(a)$

- Applications:
  - Spin models: BEG, Spherical, Potts
  - 2D vortex model (Ellis, Haven & Turkington JSP 2000, 2002)
  - Dyn phase transition in glasses (Garrahan et al PRL 2007, JPA 2009)

Method 3: Generalized canonical ensemble

(Costeniuc, Ellis, Touchette & Turkington JSP 2005, PRE 2006)

- Generalized generating function:

$$W_{n,g}(k) = \langle e^{nkA_n + ng(A_n)} \rangle$$

- Generalized free energy:

$$\lambda_g(k) = \lim_{n\to\infty} \frac{1}{n} \ln W_{n,g}(k)$$

Generalized Gärtner-Ellis Theorem

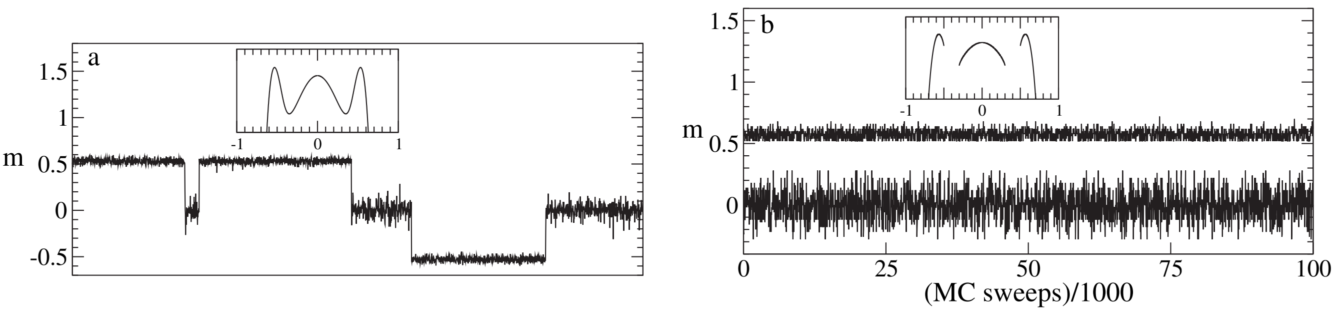
If $\lambda_g(k)$ is differentiable, then $I = \lambda_g{}^* + g$

- I nonconvex $\Rightarrow \lambda = \lambda_0$ non-differentiable
- Find g s.t. λ_g is differentiable

- Applications:
  - First-order phase transitions (Challa & Hetherington PRL 1988)
  - Potts model (Costeniuc, Ellis & Touchette PRE 2006)
  - Multifractals (Touchette & Beck JSP 2006)

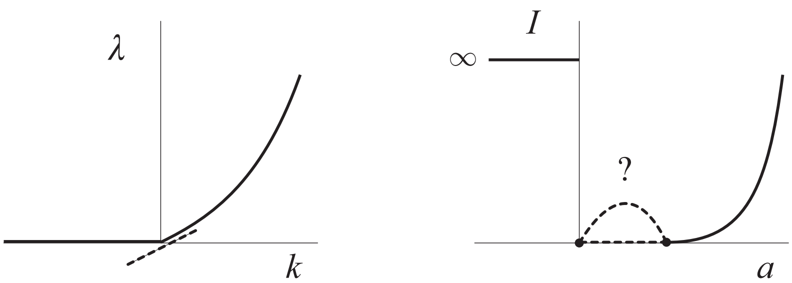
Applications

- Markov processes:
  - Finite, ergodic $\Rightarrow$ convex I
  - Sinks/absorbing states $\Rightarrow$ affine I
  - Nonconvex I
    - Infinite state space
    - Non-ergodic (Dinwoodie Ann Prob 1992, 1993)
    - Long-range correlation (?)
- Chaotic systems (Touchette & Beck JSP 2006)
- Ergodicity breaking (Mukamel et al PRL 2005, Bouchet et al PRE 2008)

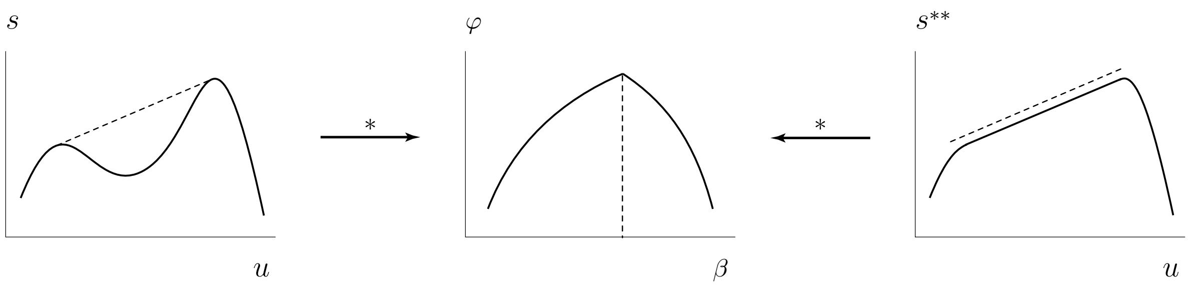


Applications (cont'd)

- Dynamical phase transitions (Garrahan et al PRL 2007, JPA 2009)
  - Fredrickson-Andersen (FA) model
  - N particle system evolving in time
  - Observable: $A_{t,N} = KS\ entropy \sim Nt$

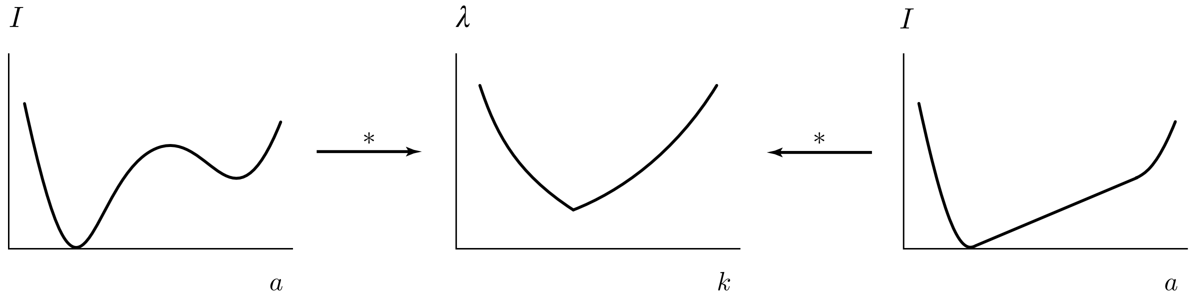


- Generic for first-order phase transitions



Nonconvex vs affine rate functions

- Nondifferentiable $\lambda(k) \Rightarrow I$ nonconvex or affine



- Perturbed free energy:

$$\lambda_\varepsilon(k) = \lim_{n\to\infty} \frac{1}{n} \ln\langle e^{nkA_n + n\varepsilon A_n^2}\rangle$$

Choose $\varepsilon = 0^-$:

- $\lambda_\varepsilon(k)$ is nondifferentiable $\Rightarrow I$ is nonconvex
- $\lambda_\varepsilon(k)$ is differentiable $\Rightarrow I$ is affine

Conclusion

- Nonconcave entropies: $s \neq \varphi^*$
- Nonconvex rate functions: $I \neq \lambda^*$
- Methods:
  - Contraction principle
  - Critical point analysis
  - Generalized canonical ensemble
- Numerical methods:

Method	Nonconvex?
Direct sampling	Y
Biased/cloning sampling	N
(Giardina, Kurchan & Peliti PRL 2006)	N
(Lecomte & Tailleur JSTAT 2007)	N
Dominant eigenvalue of generator	N
(Ground state method)	N
Wang-Landau*	Y
Multicanonical*	Y
Rugh's method*	Y

General references

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