Poles of partition functions

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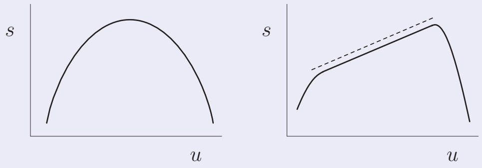
HT, Rosemary J. Harris (London), J. Tailleur (Edinburgh)
arxiv:0912.3679
Phys. Rev. E, Rapid Comm. 2010

Slides at http://www.maths.qmul.ac.uk/˜ht/talks.html

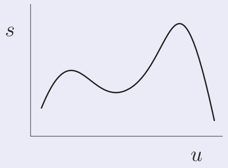
Context

- Short-range vs long-range systems
- Nonconcave entropies
- Microcanonical vs canonical
- Nonequivalence of ensembles
- First-order phase transitions

Short-range



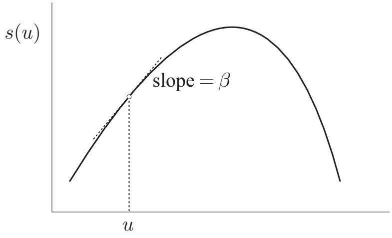
Long-range



Concave entropy

Microcanonical

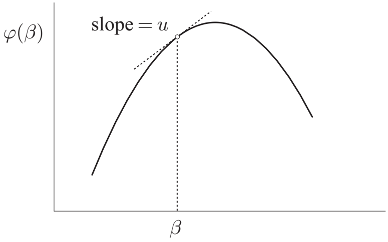
$$s(u) = \lim_{N\to\infty} \frac{1}{N} \ln \Omega_N(u)$$



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

Canonical

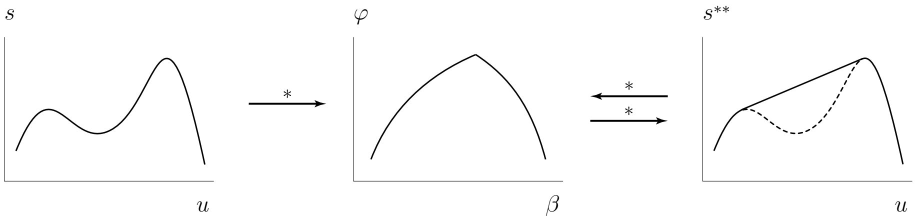
$$\varphi(\beta) = \lim_{N\to\infty} -\frac{1}{N} \ln Z_N(\beta)$$



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

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

Nonconcave entropies



Nonconcave

s

Always concave

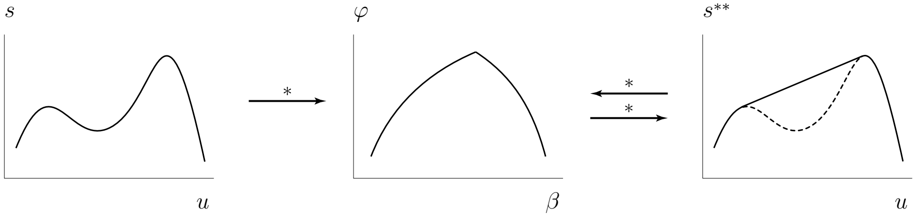
$$\varphi = s^*$$

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

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

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

Nonconcave entropies



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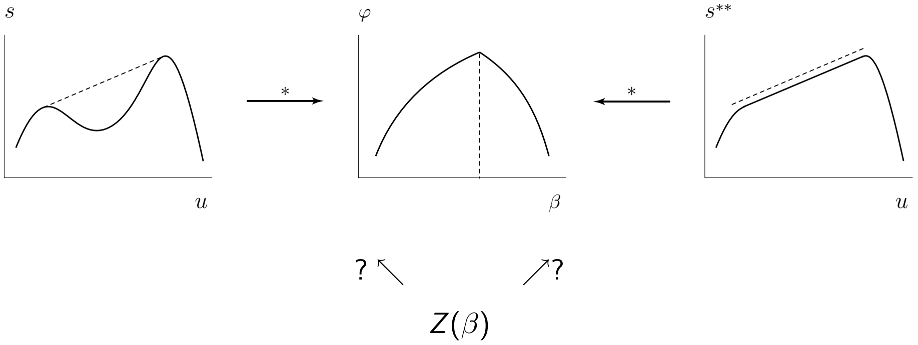
Problem

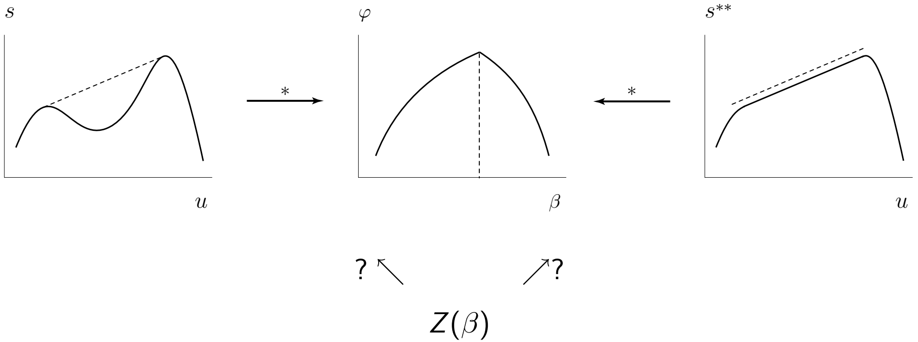
Microcanonical Canonical Microanonical



- Nonconcave/affine $s(u)$ cannot be distinguished from $\varphi(\beta)$
- Can they be distinguished from $Z(\beta)$?

Problem

Microcanonical Canonical Microanonical



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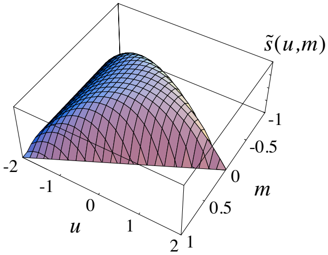
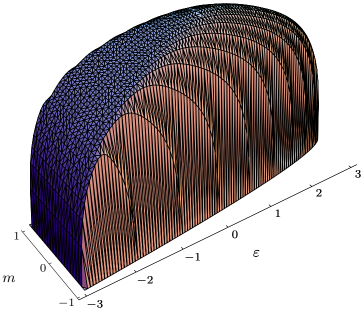
Systems with affine entropies

2D Ising model



Spherical model



Kastner & Pleimling PRL 2009

- First-order phase transitions
- Metastability
- Phase separation
- Generic for short-range systems with first-order phase transition

Result: Set-up

Inverse Laplace transform

$$\Omega(u) = \frac{1}{2\pi \mathrm{i}} \int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty} Z(\beta)\, \mathrm{e}^{\beta N u}\, \mathrm{d}\beta$$

Affine parts of $s(u) \longleftrightarrow$ Poles in series representation of $Z(\beta)$

Ansatz

$$Z(\beta) = \sum_j c_j(\beta)\, \mathrm{e}^{-N\varphi_j(\beta)}$$

- $\varphi_j(\beta)$ are smooth
- $\varphi_j(\beta)$ are independent of N
- $c_j(\beta)$ are sub-exponential in N
- $c_j(\beta)$ may have simple poles

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Result

$$s(u) = \sup_j \sup_{\beta \in \{\beta_j^*, \beta_j^\times\}} \{\beta u - \varphi_j(\beta)\}$$

- β_j^* = saddlepoints of $\beta u - \varphi_j(\beta)$
- $\beta_j^\times$ = poles of $c_j(\beta)$

Affine $s(u)$

- poles is picked up
- constant saddlepoint is picked up

Strictly concave or nonconcave $s(u)$

- no pole
- no constant saddlepoint

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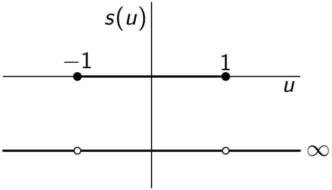
Application 1

$$Z_1(\beta) = e^{-N\beta} + e^{N\beta}$$

$$\varphi(\beta) = -|\beta|$$

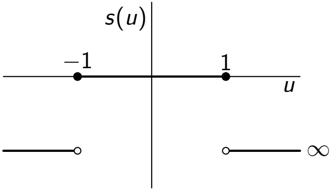
$$\Omega(u) = \delta(u+1) + \delta(u-1)$$



$$Z_2(\beta) = \frac{e^{N\beta} - e^{-N\beta}}{\beta}$$

$$\varphi(\beta) = -|\beta|$$

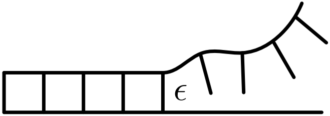
$$\Omega(u) = \begin{cases} 1 & u =\in [-1,1] \\ 0 & \text{otherwise} \end{cases}$$



Application 2: Kittel's DNA zipper model

Kittel Am. J. Phys. 1965

- Model:
  - N bonds
  - Bond energy $= \epsilon$
  - Degeneracy $= G$

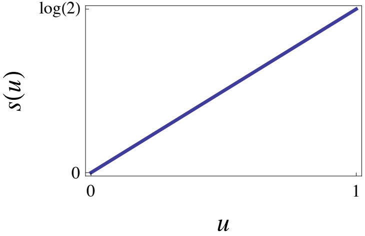


- Partition function:

$$Z(\beta) = \sum_{p=0}^{N-1} G^p\, e^{-\beta p \epsilon} \to \frac{1 - e^{-N(\beta\epsilon - \ln G)}}{N(\beta\epsilon - \ln G)}$$

- Pole: $\beta_c = \epsilon^{-1} \ln G$
- Entropy:

$$s(u) = \begin{cases} \beta_c u & u \in [0, \epsilon) \\ -\infty & \text{otherwise} \end{cases}$$



Conclusion

Main result

- New mechanism for affine entropies
- General canonical calculation method for $s(u)$
- Works for affine or concave or nonconcave $s(u)$

Applications

- Uhlenbeck-Kac model (1D gas)
- DNA models
- Markov processes (large deviation theory)

Open problems

- How to find ansatz? $Z(\beta) = \sum_j c_j(\beta)\, e^{-N\varphi_j(\beta)}$
- How to find poles?
- Transfer operator

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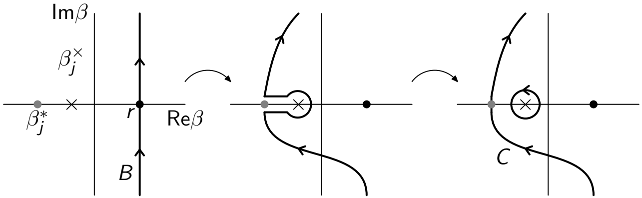
Idea of the proof

Deform Bromwich contour to S-D contour:

$$\frac{1}{2\pi \mathrm{i}}\int_B c_j(\beta)\, \mathrm{e}^{N[\beta u-\varphi_j(\beta)]}\, \mathrm{d}\beta = \frac{1}{2\pi \mathrm{i}}\int_C c_j(\beta)\, \mathrm{e}^{N[\beta u-\varphi_j(\beta)]}\, \mathrm{d}\beta + \sum \mathrm{res}$$



Approximations:

$$\frac{1}{2\pi \mathrm{i}}\int_B c_j(\beta)\, \mathrm{e}^{N[\beta u-\varphi_j(\beta)]}\, \mathrm{d}\beta \approx \underbrace{\mathrm{e}^{N[\beta_j^* u-\varphi_j(\beta_j^*)]}}_{\mathrm{e}^N \text{ S-D}} + \underbrace{\sum_\ell \sigma_{j\ell}\, \mathrm{e}^{N[\beta_{j\ell}^\times u-\varphi(\beta_{j\ell}^\times)]}}_{\mathrm{e}^N \text{ residue}}$$

- β_j^*: Saddle-point
- $\beta_{j\ell}^\times$: Poles crossed (simple)
- $\sigma_{j\ell}$: Residue parity (sign)