Poles of partition functions

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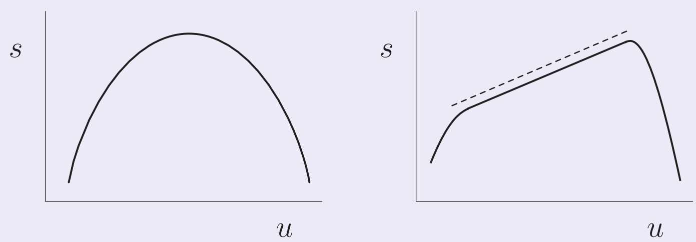
HT, Rosemary J. Harris (London), J. Tailleur (Edinburgh)
arxiv:0912.3679
Phys. Rev. E, Rapid Comm. 2010

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

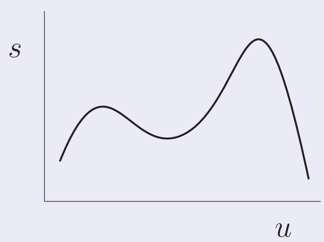
Context

- Short-range vs long-range systems
  - Gravitating particles, unscreened plasmas, free electron laser [Campa, Dauxois, Ruffo, Physics Reports 2009]
- Nonconcave entropies
- Microcanonical vs canonical
- Nonequivalence of ensembles
- First-order phase transitions

Short-range



Long-range



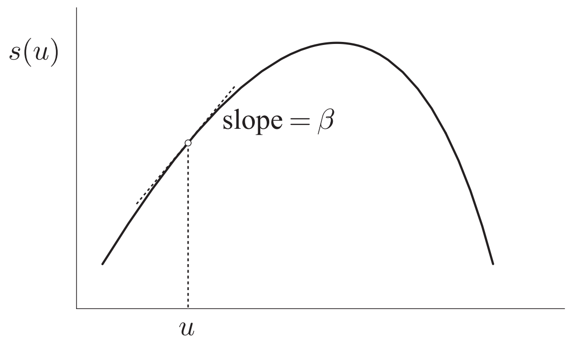
Concave entropy

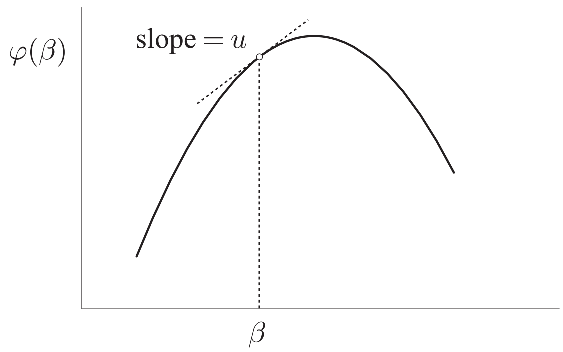
Microcanonical

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

Canonical

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



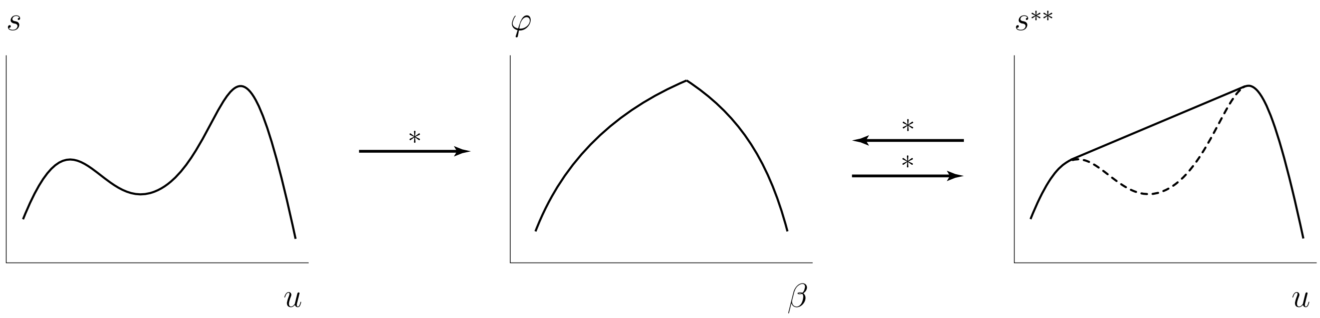


$$s(u) = \beta u - \varphi(\beta)$$
$$\varphi'(\beta) = u$$

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

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

Nonconcave entropies



Nonconcave
s

Always concave

$$\varphi = s^*$$

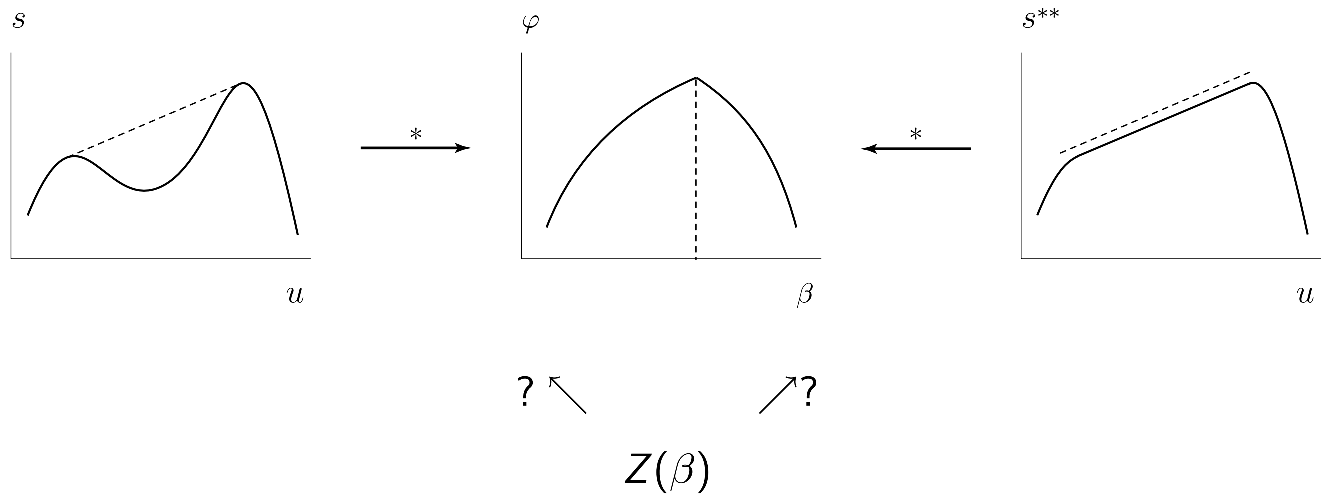
$$s \neq s^{**}$$

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

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

Problem

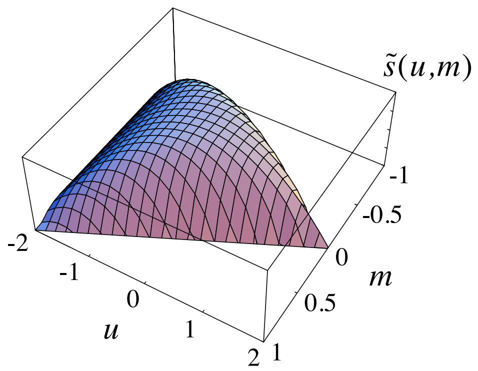
Microcanonical | Canonical | Microanonical



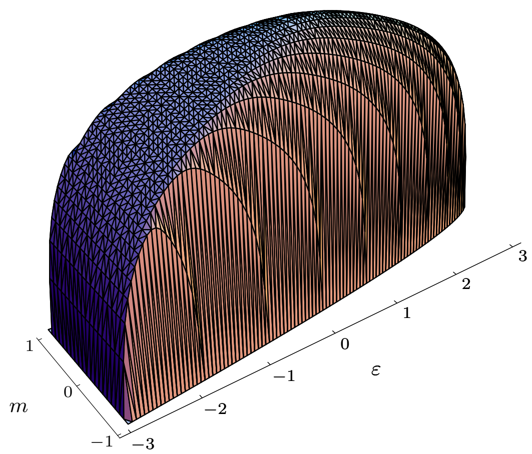
- Nonconcave/affine $s(u)$ cannot be distinguished from $\varphi(\beta)$
- Can they be distinguished from $Z(\beta)$?

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 independent of N
- $c_j(\beta)$ are sub-exponential in N
- $c_j(\beta)$ may have simple poles or branch cuts
- Decomposition is not unique

Result

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

- $\beta_j^* =$ 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 (branch cut)

Strictly concave or nonconcave $s(u)$

- no pole
- no constant saddlepoint

Application 1

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

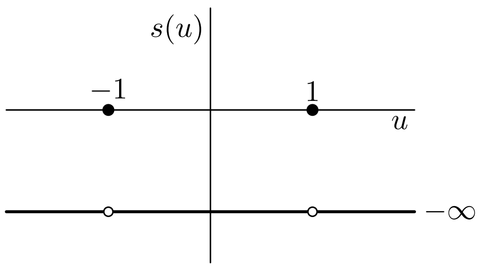
$$Z_2(\beta) = \frac{e^{N\beta} - e^{-N\beta}}{\beta}$$

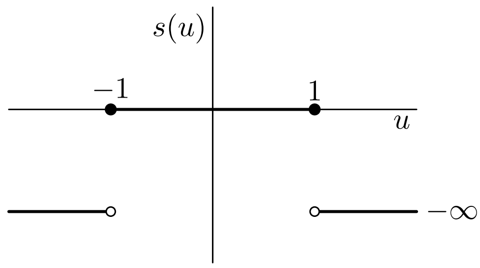
$$\varphi(\beta) = -|\beta|$$

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

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

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

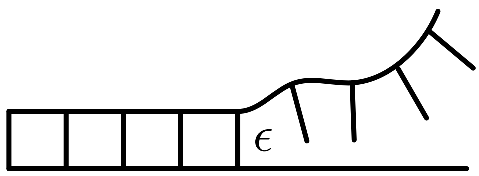




Application 2: Kittel's DNA zipper model

Kittel Am. J. Phys. 1965

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

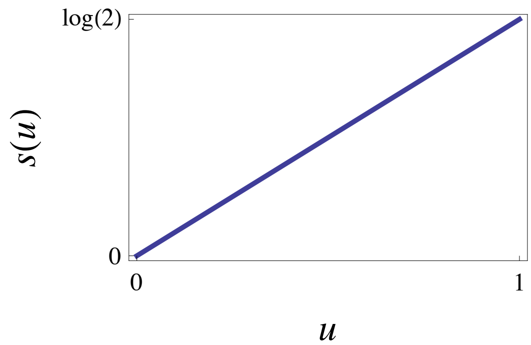


- Partition function:

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

- 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

HT, R. J. Harris, J. Tailleur, arxiv:0912.3679

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) [HT Physics Reports 2009]

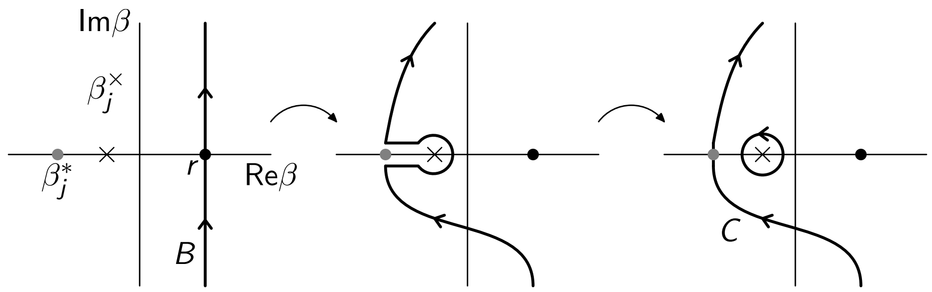
Open problems

- $d > 1$ systems
- Real vs complex poles
- Other singularities?

Idea of the proof

Deform Bromwich contour to S-D contour:

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



Approximations:

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

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

Transfer matrix expansion

$$Z(\beta) = \text{Tr}\ T_\beta^{N-1}\rho_\beta = \sum_j c_j(\beta)\, e^{-N\varphi_j(\beta)}$$

- T_β = Transfer matrix for $e^{-\beta H}$
- ρ_β = boundary condition vector
- $\varphi_j(\beta) = -\ln \xi_j(\beta)$
- $\xi_j(\beta)$ = jth eigenvalue of T_β
- $v_j(\beta)$ = jth eigenvector
- $a_j(\beta)$ = projection of ρ_β onto $v_j(\beta)$

$$c_j(\beta) = \frac{a_j(\beta)}{\xi_j(\beta)} \text{Tr}\ v_j(\beta)$$