Poles of partition functions

(Work in progress)

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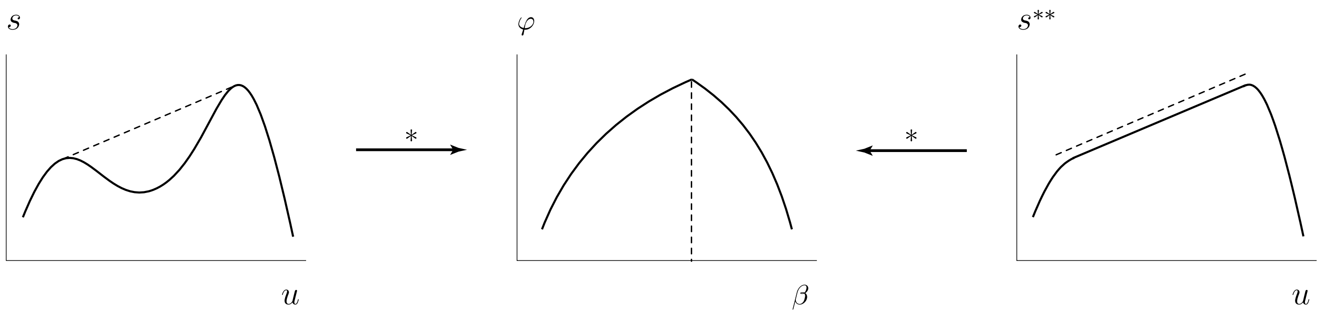
Outline

1. Context
   - Properties of $s(u)$ and $\varphi(\beta)$
   - Origin of phase transitions
2. Problem
   - Calculating $s(u)$ from $Z(\beta)$
3. Results
   - Poles of partition functions
4. Examples
5. Conclusion / open problems / conjectures



Microcanonical vs canonical

- N-particle system
- Microstate: ω
- Hamiltonian: $U(\omega)$
- Mean energy: $u = U/N$

Microcanonical

- Control parameter: u
- Density of states:

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

- Entropy:

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

Canonical

- Control parameter: β
- Partition function:

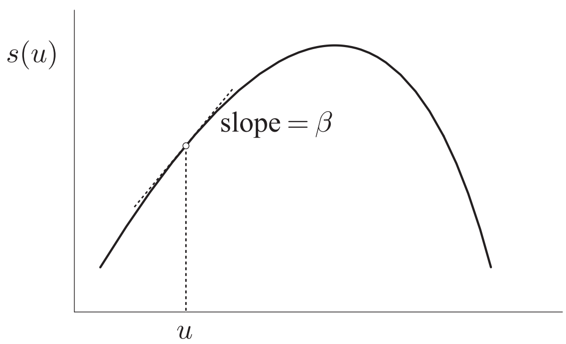
$$Z(\beta) = \int \mathrm{e}^{-\beta U(\omega)}\, \mathrm{d}\omega = \int \Omega(u)\, \mathrm{e}^{-\beta N u}\, \mathrm{d}u$$

- Free energy:

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

Concave entropy

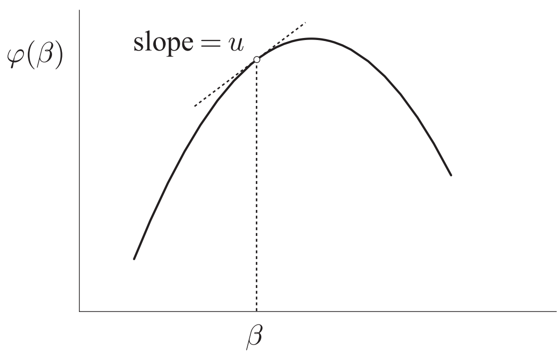
Microcanonical



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

$$s = \varphi^*$$

Canonical



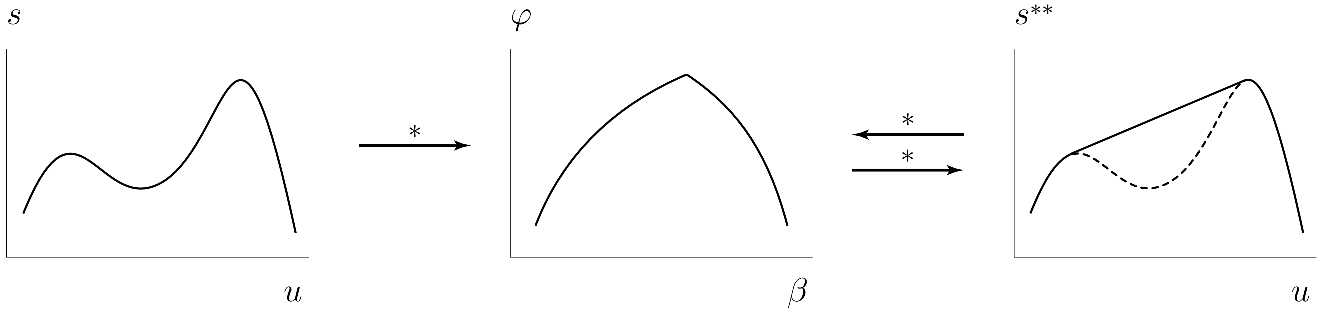
$$\varphi(\beta) = \beta u - s(u)$$
$$s'(u) = \beta$$

$$\varphi = s^*$$

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

- Legendre duality
- Equivalence of ensembles

Problem 1: Nonconcave entropies



Nonconcave
s

Always concave

$$\varphi = s^*$$

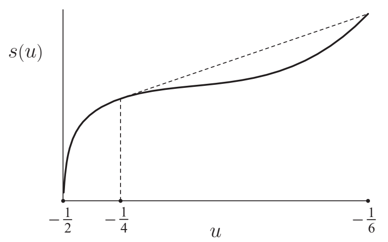
$$s \neq s^{**}$$

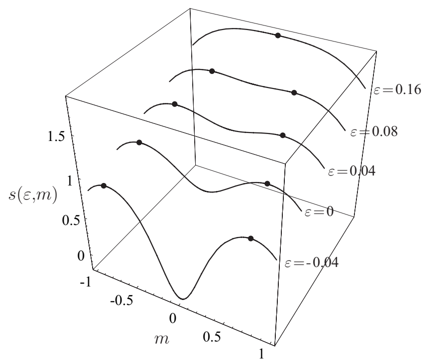
$$s^{**} = \varphi^*$$

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

Systems with nonconcave entropies

- Gravitational systems
  - Lynden-Bell, Wood, Thirring (1960-)
- Spin systems
  - Blume-Emery-Griffiths model
  - Mean-field Potts model ($q \geq 3$)
  - Mean-field ϕ^4 model
- 2D turbulence model
  - Point-vortex models, Onsagers
  - Kiessling & Lebowitz (1997)
  - Ellis, Haven & Turkington (2002)





Calculation methods

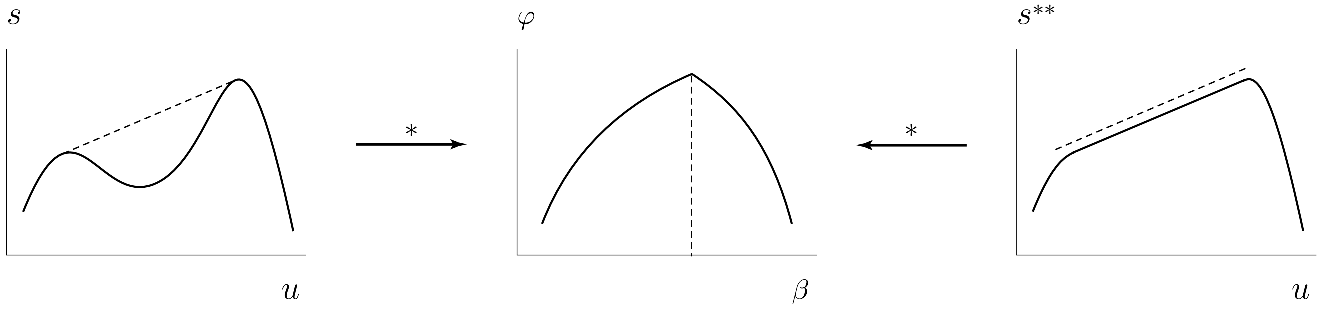
1. Contraction principle (large deviation theory)
2. Critical points of generating functions
3. Generalized canonical ensemble

Problem 2: Affine entropies

Microcanonical | Canonical | Microanonical

$Z(\beta)$

$\downarrow$



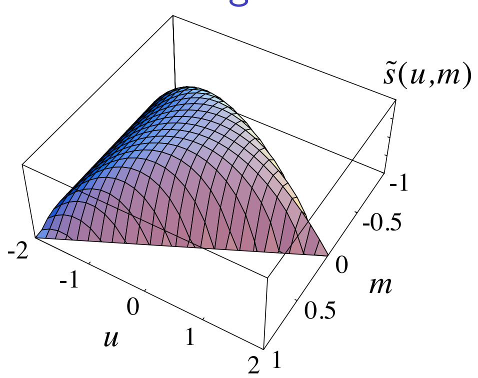
? $\nwarrow$ $\nearrow$?

$Z(\beta)$

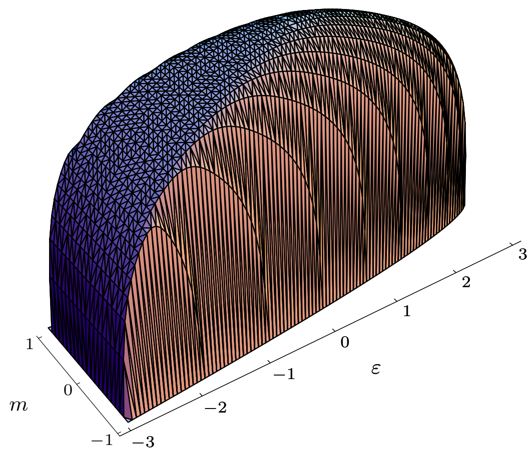
- Can we obtain $s(u)$ from $Z(\beta)$?
- Can we distinguish nonconcave/affine $s(u)$ from $Z(\beta)$?

Systems with affine entropies

2D Ising model



Spherical model



Kastner & Pleimling PRL 2009

Kastner arXiv:0909.5638

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

Starting point: Laplace transform

- Laplace transform:

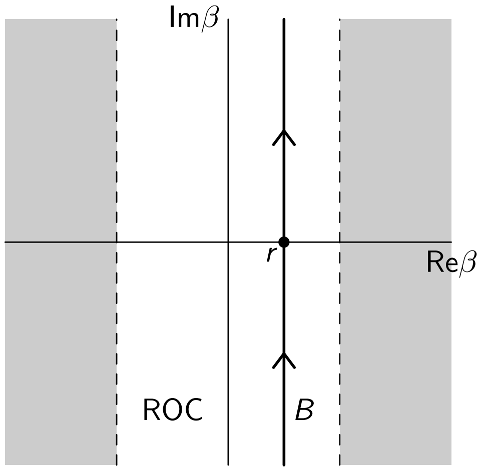
$$Z(\beta) = \int_{-\infty}^{\infty} \Omega(u)\, \mathrm{e}^{-\beta N u}\, \mathrm{d}u$$

  - Region of convergence = ROC
  - Analytic in ROC

- Inverse Laplace transform:

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

  - $r \in$ ROC
  - Bromwich contour



- Can we obtain $s(u)$ from ILT?
- Can we obtain nonconcave/affine $s(u)$ from ILT?

Standard approach: Steepest-descent approximations

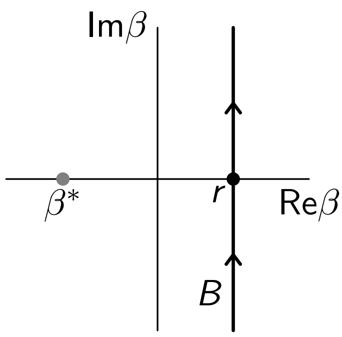
- $Z(\beta) \approx \mathrm{e}^{-N\varphi(\beta)}$
- S-D approximation:

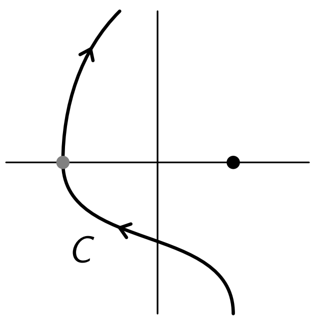
$$\begin{aligned}
\Omega(u) &\approx \frac{1}{2\pi \mathrm{i}} \int_B \mathrm{e}^{N[\beta N u - \varphi(\beta)]}\, \mathrm{d}\beta \\
&= \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{e}^{N[\beta u - \varphi(\beta)]}\, \mathrm{d}\beta \\
&\approx \mathrm{e}^{N[\beta^* u - \varphi(\beta^*)]}
\end{aligned}$$

  - Saddle-point: $\varphi'(\beta^*) = u$
  - S-D contour: $\mathrm{Im}\{\beta u - \varphi(\beta)\} = 0$

- Entropy:

$$s(u) = \beta^* u - \varphi(\beta^*) = \inf_\beta \{\beta u - \varphi(\beta)\}$$





$s(u)$ obtained is necessarily concave

Two examples

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

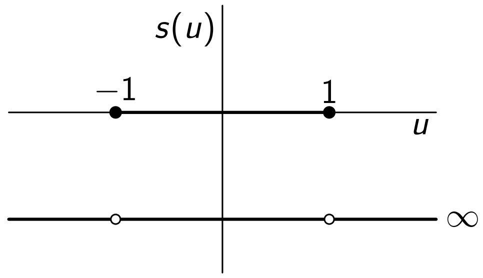
$$Z_2(\beta) = \frac{\mathrm{e}^{N\beta} - \mathrm{e}^{-N\beta}}{\beta}$$

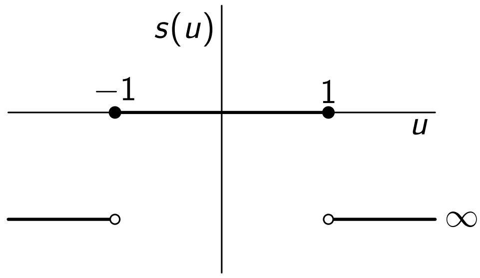
$$\varphi(\beta) = -|\beta|$$

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

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

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





- Work with $Z(\beta)$ not $\varphi(\beta)$

New approach: Poles of partition functions

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

No pole

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

Poles

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

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

Decomposition is not unique

Effect of poles

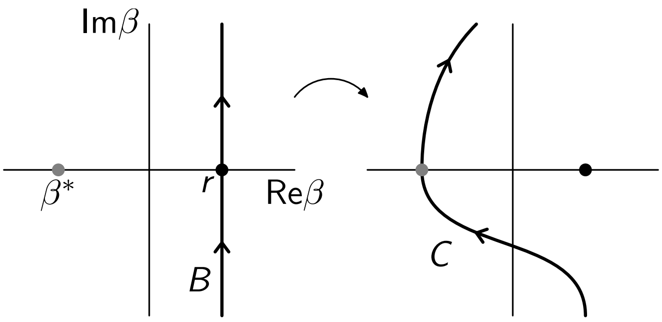
1. Distribute ansatz in ILT:

$$\Omega(u) = \sum_j \frac{1}{2\pi \mathrm{i}} \int_B c_j(\beta)\, \mathrm{e}^{N[\beta u - \varphi_j(\beta)]}\, \mathrm{d}\beta.$$

2. Deform Bromwich contour to S-D contour:

Case A: No crossing of poles:

$$\frac{1}{2\pi \mathrm{i}} \int_B c_j(\beta)\, \mathrm{e}^{N[\beta u - \varphi_j(\beta)]}\, \mathrm{d}\beta = \frac{1}{2\pi \mathrm{i}} \int_C c_j(\beta)\, \mathrm{e}^{N[\beta u - \varphi_j(\beta)]}\, \mathrm{d}\beta$$
$$\approx \mathrm{e}^{N[\beta_j^* u - \varphi(\beta_j^*)]}$$

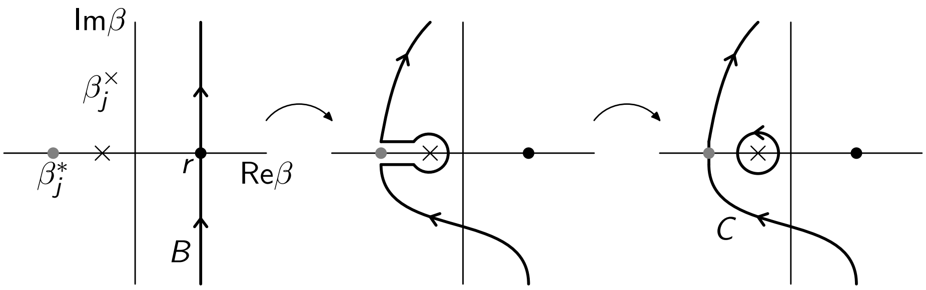


Effect of poles (cont'd)

2. Deform Bromwich contour to S-D contour:

Case B: Crossing of poles:

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



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)

Effect of poles (cont'd)

3. Gather approximations:

$$\Omega(u) \approx \sum_j e^{N[\beta_j^* u - \varphi(\beta_j^*)]} + \sum_\ell \sigma_{j\ell}\, e^{N[\beta_{j\ell}^\times u - \varphi(\beta_{j\ell}^\times)]}$$

   - Possible cancellation of terms

4. Take largest term (Laplace approximation):

$$\Omega(u) \approx \exp\left(N \sup_j \sup_{\beta\in B_j} \{\beta u - \varphi_j(\beta)\}\right)$$

   - B_j = set of non-cancelling saddlepoints β_j^* and poles $\beta_{j\ell}^\times$

Final result

$$s(u) = \sup_j \sup_{\beta\in B_j} \{\beta u - \varphi_j(\beta)\}$$

Concavity of $s(u)$

$$s(u) = \sup_j \sup_{\beta\in B_j} \{\beta u - \varphi_j(\beta)\}$$

Affine $s(u)$

- max over B_j picks up a pole
- max over B_j picks up a saddlepoint that is constant as a function of u
  - Farago JSP 2002
  - Kastner arXiv:0909.5638

Strictly concave or nonconcave $s(u)$

- max over B_j picks up neither a pole nor a constant saddlepoint

No poles

$$s(u) = \sup_j \{\beta_j^* u - \varphi_j(\beta_j^*)\} = \sup_j \inf_\beta \{\beta u - \varphi_j(\beta)\}$$

Application: Kittel's DNA zipper model

Kittel Am. J. Phys. 1965

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

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

- Decomposition:

$$Z(\beta) = \frac{1}{1 - e^{-(\beta - \beta_c)\epsilon}} - \frac{e^{-N(\beta\epsilon - \ln G)}}{1 - e^{-(\beta - \beta_c)\epsilon}}$$

- Poles: $e^{\beta\epsilon} = G$
  - Infinite number of poles
  - How to deform contour?

Application: Kittel's DNA zipper model (cont'd)

Observations

- Complex poles come from discrete energy levels
- $u = U/N \to$ continuous variable in thermo limit
- Study $Z(\beta)$ in thermo limit

- Thermo-limit partition function:

$$\begin{aligned} Z(\beta) &= \sum_{p=0}^{N-1} G^p \, e^{-\beta p \epsilon} = \sum_r e^{-N(\beta r \epsilon - r \ln G)}, \qquad r = p/N \\ &\to \int_0^1 e^{-Nu(\beta\epsilon - \ln G)} \, du = \frac{1 - e^{-N(\beta\epsilon - \ln G)}}{N(\beta\epsilon - \ln G)} \end{aligned}$$

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

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

Large deviation generalization

Statistical mechanics	Large deviation theory	
$u = \dfrac{U}{N}$	A_n	Random variable
$\Omega(u)$	$P(A_n = a)$	Prob distribution
$Z(\beta)$	$G(k) = \langle \mathrm{e}^{nkA_n} \rangle$	Generating function
$\Omega(u) \approx \mathrm{e}^{Ns(u)}$	$P(A_n = a) \approx \mathrm{e}^{-nI(a)}$	Rate function
$Z(\beta) \approx \mathrm{e}^{-N\varphi(\beta)}$	$G(k) \approx \mathrm{e}^{n\lambda(k)}$	Scaled cumulant generating function
$s(u) = \inf_\beta \{\beta u - \varphi(\beta)\}$	$I(a) = \sup_k \{ka - I(a)\}$	Gärtner-Ellis Thm

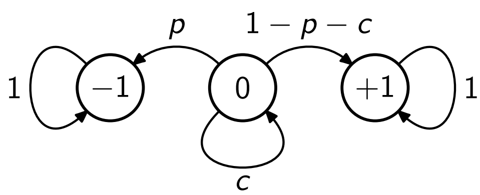
Application: Markov processes

- Markov process: $X_i \in \{-1, 0, 1\}$

$$S_n = \frac{1}{n}\sum_{i=1}^{n} X_i, \qquad p(x_1, \ldots, x_n) = p(x_1)\prod_{i=2}^{n} \pi(x_n|x_{n-1})$$

- Transition matrix:

$$\Pi = \begin{pmatrix} 1 & p & 0 \\ 0 & c & 0 \\ 0 & 1-p-c & 1 \end{pmatrix}$$



  - Absorbing states: ± 1
- Generating function: $G(k) = \langle \mathrm{e}^{nkS_n} \rangle$
- Transfer operator:

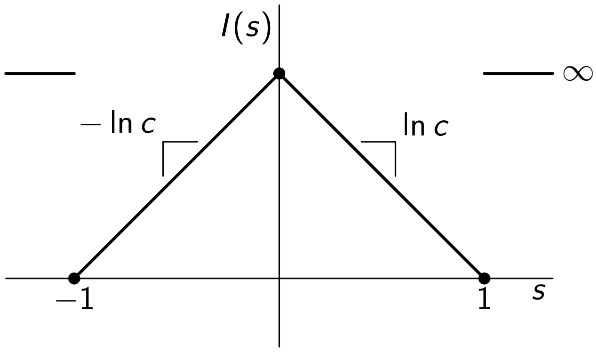
$$\Pi_k = \begin{pmatrix} e^{-k} & pe^{-k} & 0 \\ 0 & c & 0 \\ 0 & (1-p-c)e^{k} & e^{k} \end{pmatrix}$$

Application: Markov processes (cont'd)

- Generating function:

$$W_n(k) = \frac{e^{-nk}}{1 - ce^k} + \frac{e^{nk}}{e^k - c} + \frac{e^{n \ln c}(1 - e^k)(1 - ce^k - p - e^k p)}{c - e^k - c^2 e^k + ce^{2k}}$$

  - Infinite number of poles
  - Real poles: $k = \pm \ln c$
  - Keep only the real poles
- Rate function:



Conclusion / open problems / conjectures

Main result

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

Open problems

- What to do with complex poles?
- How to find ansatz? $Z(\beta) = \sum_j c_j(\beta)\, e^{-N\varphi_j(\beta)}$
- How to find poles?
  - Look at eigenvectors and eigenvalues of transfer operator

Conjectures

- Complex poles related to discreteness of energy levels
- Only real poles are "essential" in thermodynamic limit
- Short-range systems with 1st PT $\leftrightarrow$ real pole at β_c

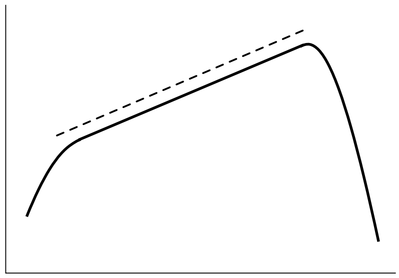
Last result

If

- $s(u)$ is affine over (u_l, u_h):

$$s(u) = s(u_l) + \beta_c (u - u_l)$$

- $\Omega(u) \approx \mathrm{e}^{Ns(u)}$



Then

$$Z(\beta) = \int_{-\infty}^{u_l} \Omega(u)\, \mathrm{e}^{-N\beta u}\, \mathrm{d}u + \underbrace{\int_{u_l}^{u_h} \Omega(u)\, \mathrm{e}^{-N\beta u}\, \mathrm{d}u}_{\propto \frac{1}{\beta - \beta_c}} + \int_{u_h}^{\infty} \Omega(u)\, \mathrm{e}^{-N\beta u}\, \mathrm{d}u$$

$s(u)$ affine $\Rightarrow$ $Z(\beta)$ admits an expansion with a pole