Thermodynamics of histories for kinetically constrained models

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Outline

- Phenomenology of kinetically constrained models (KCMs)
- Relevant order parameters for space-time trajectories
- Results: mean-field/ finite dimensions
- Conclusion

Phenomenology of KCMs

- Spin models on a lattice, with specific dynamical rules
  - $s_i = 1$, $n_i = 1$: "mobile" particle - region of low density
  - $s_i = -1$, $n_i = 0$: "blocked" particle - region of high density
  - $H = \sum_i n_i \rightarrow < n >_{eq} = c = 1/(1 + e^{\beta})$
- Fredrickson-Andersen (FA) model in 1 dimension: a spin can flip only if at least one of its nearest neighbours are in the mobile state.
  "Facilitation": mobile low-density regions facilitate local rearrangements.
  [Ritort, Sollich, 2003]

Phenomenology of KCMs

- East model ($1d$): a spin can flip only if its right neighbour is in the mobile state.
- Kob-Andersen (KA) model: the particle number is conserved: $\sum_i n_i = 1 - \rho$.
- In the context of glassy dynamics:
  - ”dynamic heterogeneity” is put by hand: mobile particles vs blocked particles
  - facilitation mimicks steric effects in amorphous solids (molecular glasses, colloids, jammed materials,..)
  - slow relaxation (stretched exponentials)
  - these systems can be brought out of equilibrium by a quench in T and exhibit aging.

Phenomenology of KCMs

- Growing of dynamic spatial correlations: particles are dynamically correlated (cooperative) on a lengthscale ξ, not related to static correlations.
  e.g: KA model, $\xi(\rho) \propto exp(exp(C/(1-\rho)))$, measurable through 4-points spatio-temporal correlation functions.
- Absence of a dynamical phase transition (”glass transition”) at $T > 0$, but strong finite-size effects around $T = 0$ ($\rho = 1$). e.g: KA model in 3d:
  $1 - \rho^*(L) \propto 1/\ln(\ln L)$.

Phenomenology of KCMs

- However: in the FA model, configurations are split into 2 distinct partitions.
  - $\downarrow\uparrow\downarrow \rightleftharpoons \downarrow\downarrow\downarrow$ is forbidden
  - $n_i = 0$ for all i is a partition of its own.
  - all other configurations $(2^N - 1)$: "high-T" partition, active configurations.
  - $\rightarrow$ FA is reducible - "effectively" irreducible
  - $\rightarrow$ (even weak) reducibility is crucial in the study of phase-space trajectories.
- How to classify trajectories? How to quantify dynamical complexity?
- Quantities like a dynamical entropy (Kolmogorov-Sinai entropy h_{KS}) are likely to be relevant.

Relevant order parameters for space-time trajectories

- Ruelle formalism for continous-time Markov dynamics
- Observable: $K(t)$: number of flips between 0 and t.
- Master equation:
  $\frac{\partial P}{\partial t}(C,t) = \sum_{C'} W(C' \to C)P(C',t) - r(C)P(C,t)$, where
  $r(C) = \sum_{C'} W(C \to C')$
- $\hat{P}(C,s,t) = \sum_K e^{-sK} P(C,K,t) \to \partial_t \hat{P} = \mathbb{W}_K \hat{P}$, where
  $\mathbb{W}_K(s)(C,C') = e^{-s} W(C' \to C) - r(C)\delta_{C,C'}$.
- Generating function of K:
  $Z_K(s,t) = \sum_C \hat{P}(C,s,t) =< e^{-sK} >$. For $t \to \infty$,
  $Z_K(s,t) \simeq e^{t\psi_K(s)}$: $\psi_K(s)$ is the largest eigenvalue of
  $\mathbb{W}_K(s)$.

Relevant order parameters for space-time trajectories

- Average activity: $\frac{<K>(s,t)}{Nt} \underset{t\to\infty}{=} -\frac{1}{N}\psi'_K(s)$.
  Average density of particles at fixed s:
  $\rho_K(s) = \lim_{t\to\infty} \frac{1}{Z_K(s,t)} \sum_{\text{histories}} e^{-sK(\text{history})}\rho(t)$.
- Analogy:
  - space of configurations, fixed β:
    $Z(\beta) = \sum_C e^{-\beta H} \simeq e^{-Nf(\beta)}$, $N \to \infty$.
  - space of trajectories, fixed s:
    $Z_K(s,t) = \sum_{C,K} e^{-sK} P(C,K,t) \simeq e^{-tf_K(s)}$, $t \to \infty$.
  - $f_K(s) = -\psi_K(s)$: free energy for trajectories
  - $\rho_K(s)$, $\frac{<K>(s,t)}{Nt}$: activity/chaoticity.
- Active phase: $< K > (s,t)/(Nt)$, $\rho_K(s) > 0$: $s < 0$.
  Inactive phase: $< K > (s,t)/(Nt)$, $\rho_K(s) = 0$: $s > 0$.

Relevant order parameters for space-time trajectories

- Similar order parameters can be defined for the observable $Q_+(t) = \sum_{n=0}^{K-1} \ln \frac{W(C_n \to C_{n+1})}{r(C_n)} = \ln \mathrm{Prob}(\mathrm{history}(0 \to t))$.
- $Z_{dyn}(s,t) = \sum_{\mathrm{histories}} \left[\mathrm{Prob}(\mathrm{history})\right]^{1-s} =< e^{-sQ_+} > \underset{t\to\infty}{\sim} e^{t\psi_+(s)}$
- $\psi_+(s)$: topological pressure; $\rho_+(s)$: analog of $\rho_K(s)$.
- $h_{KS} = \psi'_+(s=0) = \lim_{t\to\infty} -\frac{<Q_+(t)>}{t}$: Kolmogorov-Sinai entropy.
    - $h_{KS} = 0$: one possible trajectory in configuration space.
    - $h_{KS} > 0$: many possible trajectories in configuration space.

Results: Mean-Field FA

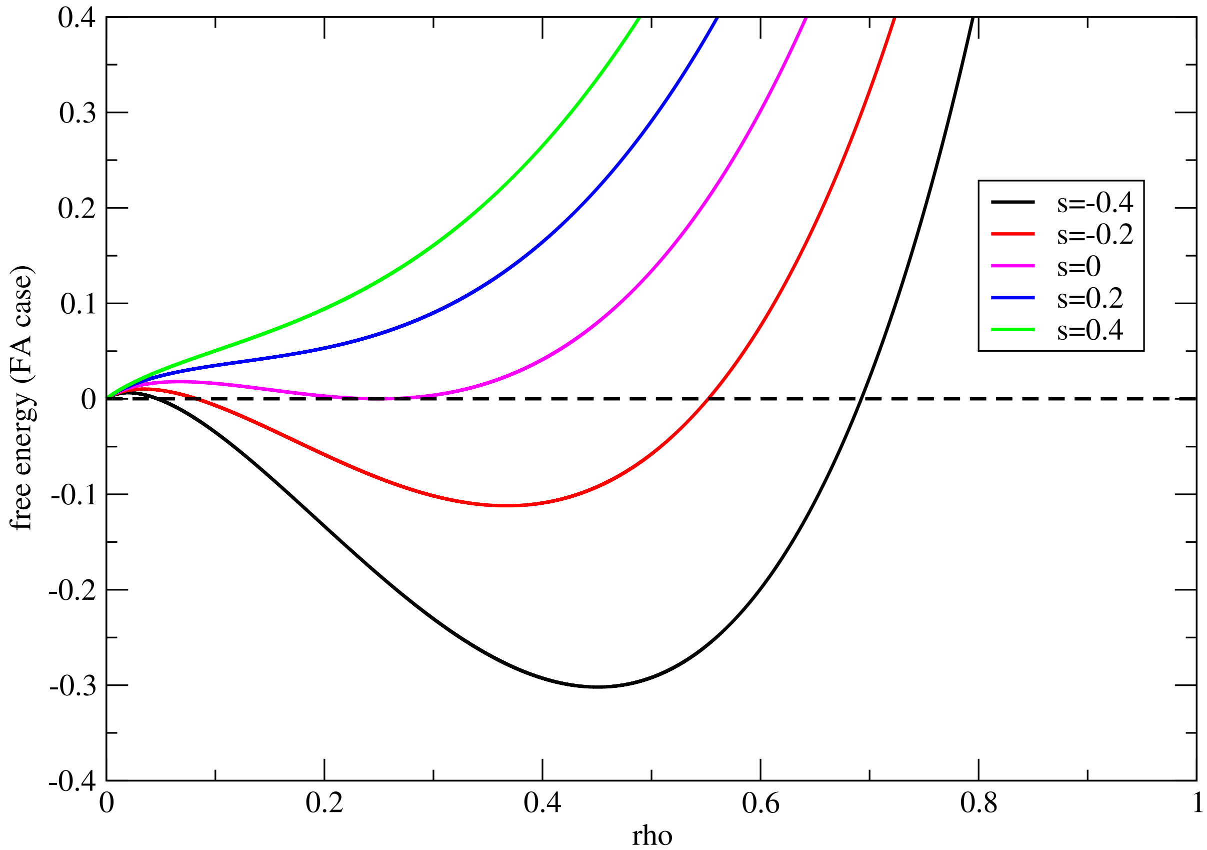
- $W_i(0 \to 1) = k' \frac{n}{N}$, $W_i(1 \to 0) = k \frac{n-1}{N}$, $n = \sum_i n_i$.
- Equilibrium distribution: $P_{eq}(n) = \frac{1}{Z} C_N^n e^{-\beta n}$, where $Z = (1+\zeta)^N$, $\zeta = \frac{k'}{k} = e^{-\beta}$.
- Symmetrization of $\mathbb{W}_K$: $\tilde{\mathbb{W}}_K = Q^{-1} \mathbb{W}_K Q$, with $Q(C, C') = P_{eq}^{1/2}(C) \delta_{C,C'}$.
- $\tilde{\mathbb{W}}_K(n, n') = e^{-s}(W_+(n-1)W_-(n))^{1/2} \delta_{n',n-1} + e^{-s}(W_+(n)W_-(n+1))^{1/2} \delta_{n',n+1} - r(n)\delta_{n,n'}$
- $\psi_K(s)$: largest eigenvalue of $\mathbb{W}_K$ can be calculated using: $\psi_K(s) = \max_P \frac{<P|\tilde{\mathbb{W}}_K|P>}{<P|P>}$

Results: Mean-Field FA

- Assuming a homogeneous profile $\rho = \frac{n}{N}$: variational principle for $\psi_K(s)$, involving a Landau-Ginzburg free energy $F_K(\rho, s)$:
  $\frac{1}{N} f_K(s) = -\frac{1}{N}\psi_K(s) = \min_{\rho} F_K(\rho, s)$, with
  $$F_K(\rho, s) = -2\rho e^{-s}(\rho(1-\rho)kk')^{1/2} + k'\rho(1-\rho) + k\rho^2$$
- Minima of $F_K(\rho, s)$ at fixed s:
  - $s > 0$: inactive phase, $\rho_K(s) = 0$, $\psi_K(s) = 0$.
  - $s = 0$: coexistence $\rho_K(0) = 0$ and $\rho_K(0) = \rho^*$, $\psi_K(0) = 0$, $\rightarrow$ first order phase transition.
  - $s < 0$: active phase, $\rho_K(s) > 0$, $\psi_K(s) > 0$.

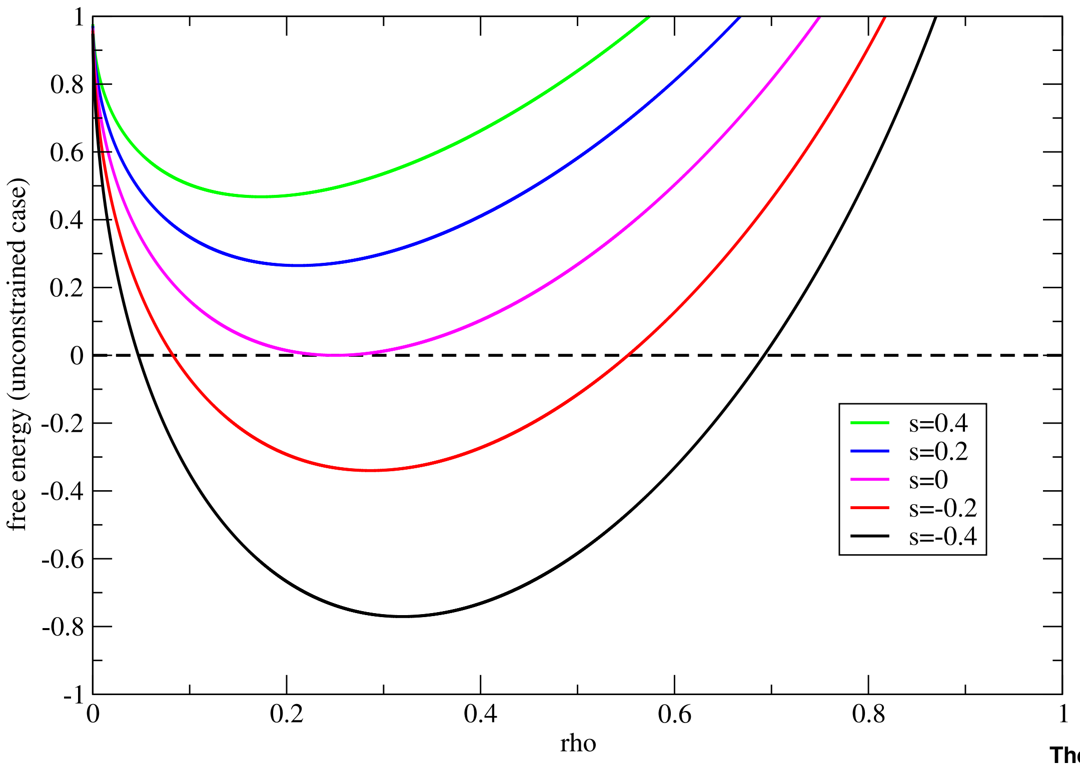
Results: Mean-Field FA

- $F_K(\rho, s)$ for different values of s:



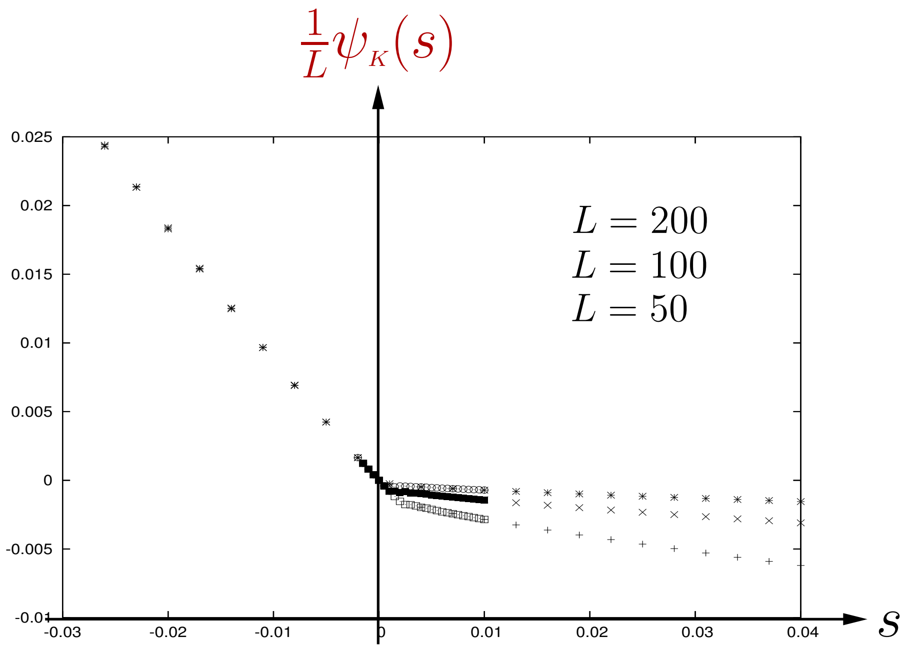
Results: Mean-Field unconstrained model

- $W_i(0 \to 1) = k'$, $W_i(1 \to 0) = k$, for all i
- $F_K(\rho, s) = -2e^{-s}(\rho(1-\rho)kk')^{1/2} + k'(1-\rho) + k\rho$
- No first-order phase transition.



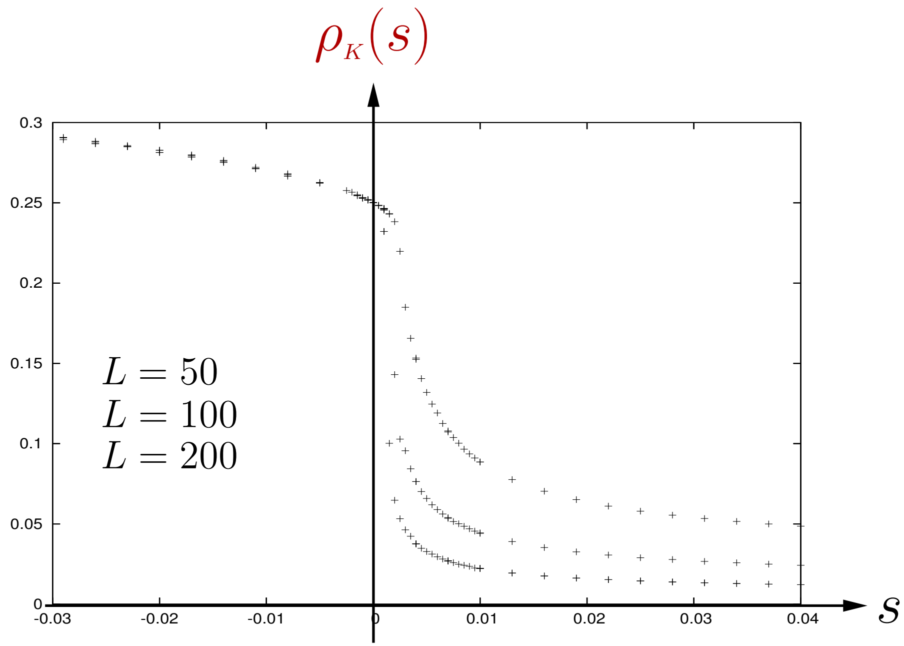
Results in finite dimensions

- Numerical solution using the algorithm of Giardina, Kurchan, Peliti for large deviation functions.
- First-order phase transition for the FA model in 1d.



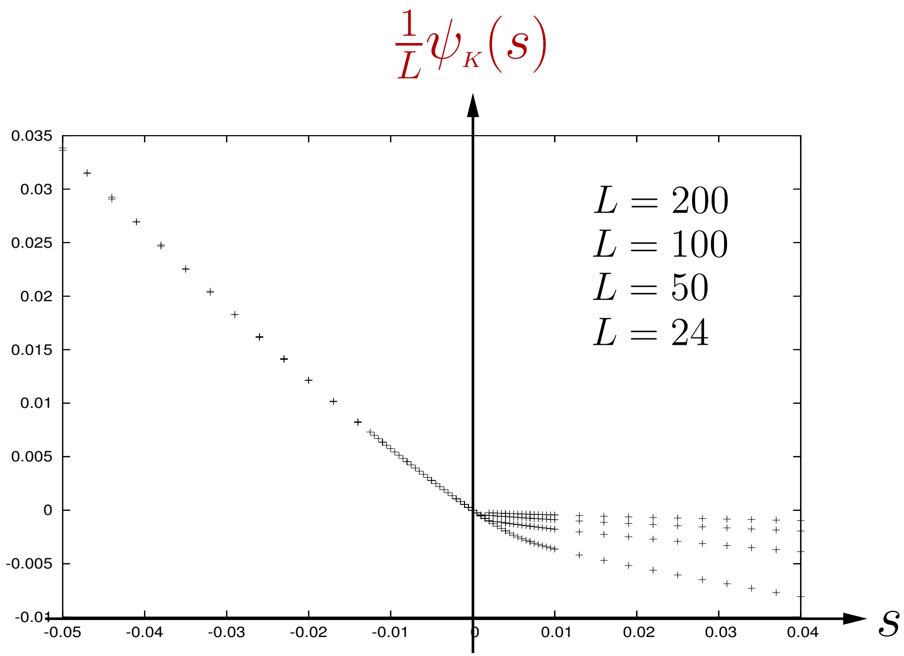
Results in finite dimensions

- $\rho_K(s)$ for the FA model in 1d.



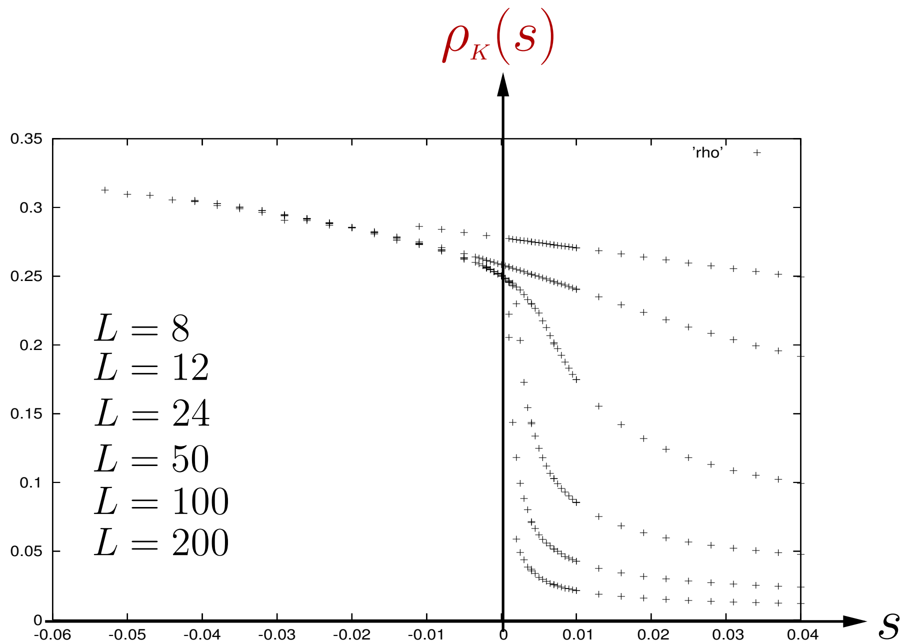
Results in finite dimensions

- First-order phase transition for the East model.



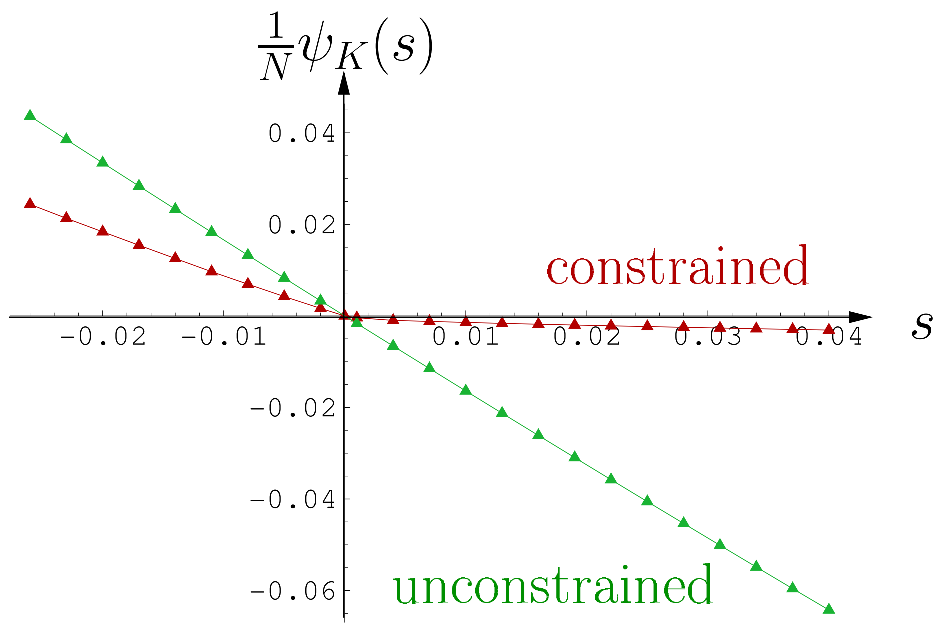
Results in finite dimensions

- $\rho_K(s)$ for the East model.



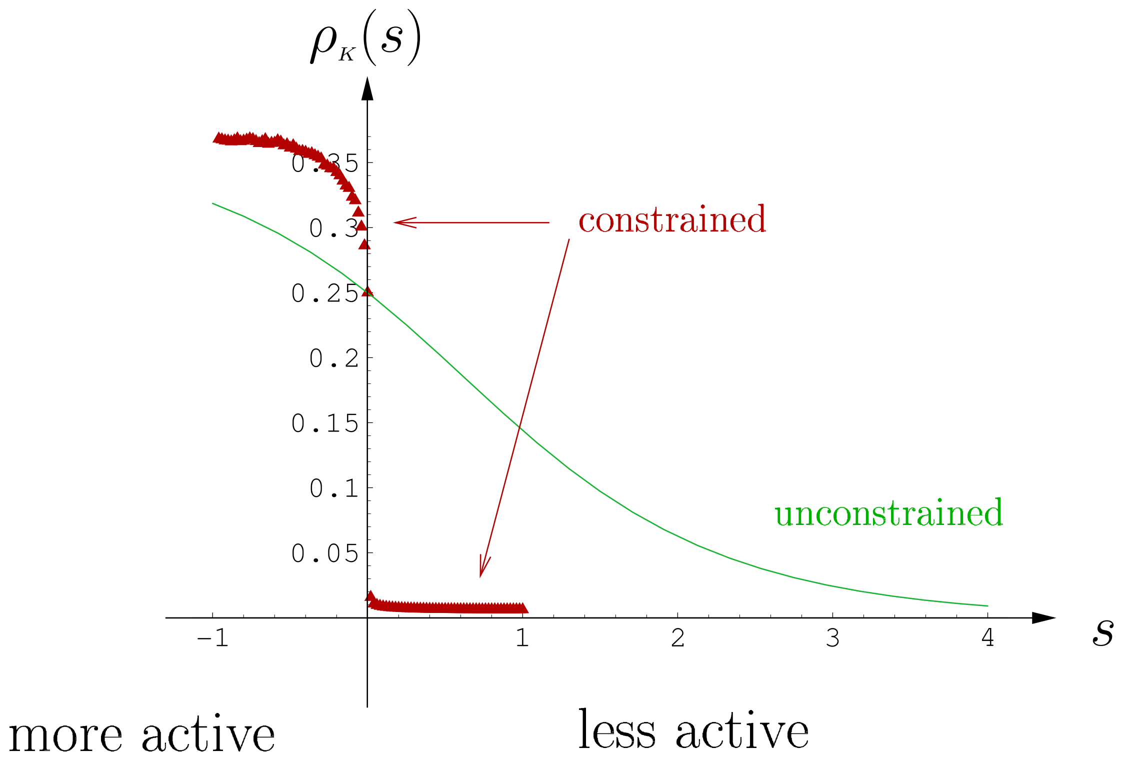
Results in finite dimensions

- Comparison between 1d FA model and unconstrained model $A \xrightarrow{k} \emptyset$, $\emptyset \xrightarrow{k'} A$.



Results in finite dimensions

- $\rho_K(s)$ for the 1d FA model and $A \xrightarrow{k} \emptyset$, $\emptyset \xrightarrow{k'} A$.



- The existence of the first-order phase transition -and coexistence of active and inactive phases- relies on the reducible character of the dynamical model.
- e.g: AA model
  - $\emptyset A \underset{}{\overset{D}{\rightleftharpoons}} A\emptyset$, $AA \xrightarrow{k} \emptyset\emptyset$, $\emptyset\emptyset \xrightarrow{k'} AA$
  - Solvable model in 1d using free fermions for $2D = k + k' \rightarrow$ no first-order phase transition.

Conclusions

- Large deviation functions of generating functions in trajectories space provide useful order parameters that probe active/inactive phases. s plays the role of a "chaoticity" temperature.
- KCMs which are (even weakly) reducible show a first-order phase transition at $s = 0$. In a real system, coexistence between inactive and active states induce the slowing down of the dynamics.
- Possible link between ξ -dynamical correlation length- and moments of $K(t)$.
- Look in more detail into specific features of glassiness: strong glass (FA) vs fragile glass (East).
- Study a more realistic glassy system in trajectory space.