Large deviations, metastability, and effective interactions

Robert Jack (University of Bath)

Warwick workshop : metastability / KCMs, Jan 2016

Thanks to:
Peter Sollich (Kings College London)
Juan Garrahan (Nottingham) and David Chandler (Berkeley)
Fred van Wijland, Vivien Lecomte (Paris-Diderot)
Ian Thompson (Bath) and Yael Elmatad (Tapad)

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(Glass transitions?)

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(Examples: symmetric simple exclusion process, $1d$ Ising model)

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Conditioned set of trajectories can be described* by "auxiliary" (driven) process with "effective interactions"

(* Terms and conditions apply)

[RML Evans 2003, Maes & Netocny 2008, RLJ & Sollich 2010, Touchette & Chetrite 2015]

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$$\partial_t p(\mathcal{C}, t) = \sum_{\mathcal{C}' \neq \mathcal{C}} [p(\mathcal{C}', t) W(\mathcal{C}' \to \mathcal{C}) - p(\mathcal{C}, t) W(\mathcal{C} \to \mathcal{C}')]$$

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Write

$\partial_t p^{\mathcal{C}}(t) = \mathbb{W}_0 p^{\mathcal{C}}(t)$

($\mathbb{W}_0$ is the (forward) generator)

($p^{\mathcal{C}}$ is a discrete probability distribution over $\mathcal{C}$)

Large deviations…

[Lebowitz-Spohn, Bodineau-Derrida, Lecomte-van Wijland, etc]

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Finally end up with

$$\partial_t p^{\mathcal{C}}(s,t) = \mathbb{W}(s) p^{\mathcal{C}}(s,t)$$

... and $\mathbb{W}(s)$ typically has a simple representation

Auxiliary process

[following RLJ-Sollich 2010]

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Define $\mathbb{W}^{\mathrm{aux}} = u^{-1}\mathbb{W}(s)u - \psi(s)$
with

$\psi(s)$: largest eigenvalue of $\mathbb{W}(s)$

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Then $\mathbb{W}^{\rm aux}$ is the (transposed) generator for the auxiliary process [for conditioning $K/t_{\rm obs} \approx -\psi'(s)$]

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This is an *explicit construction* of the auxiliary process that mimics the conditioning

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The transition rates for the auxiliary process are
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[?? can we do this on infinite lattices ?? see later]

Effective interactions

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Some interesting cases:

1. Exclusion processes (SSEP and ASEP)

2. East model

3. 1d Ising model

4. Model sheared systems

Exclusion processes

Particles on periodic $1d$ lattice, at most one per site, attempt to hop right (or left) with rate $1 + a_0$ (or $1 - a_0$).

Joint conditioning on activity (bias s) and current (bias h)

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$$\mathbb{W}(s,h) = \sum_i \mathrm{e}^{-s+h}(1+a_0)\sigma_i^- \sigma_{i+1}^+ + \mathrm{e}^{-s-h}(1-a_0)\sigma_i^+ \sigma_{i+1}^- - 2n_i(1-n_i)$$

$$n_i = \sigma_i^+ \sigma_i^-$$

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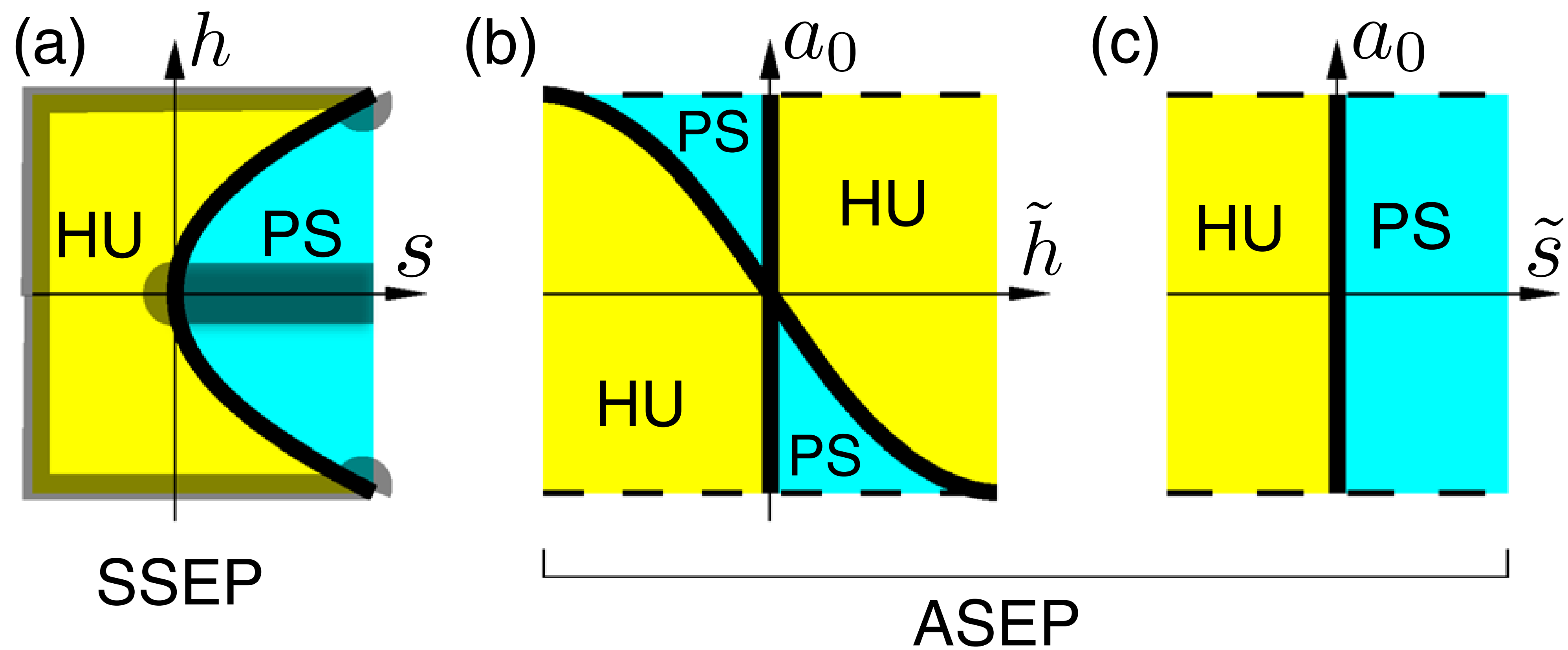
[RLJ, Thompson, Sollich, PRL **114,** 060601 (2015)]



HU: hyperuniform state

PS: “phase-separated” (inhomogeneous) state

Hyperuniformity

[Torquato and Stillinger, 2003-]

In HU states, the variance of the number of points in a region of volume R^d scales as

$$\langle \delta n(R^d)^2 \rangle \sim R^{d-1}$$

In ‘normal’ equilibrium states

$$\langle \delta n(R^d)^2 \rangle \sim \kappa R^d$$

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HU states have strong suppression of large-scale density fluctuations…

… jammed particle packings, biological systems, novel photonic materials, galaxies…

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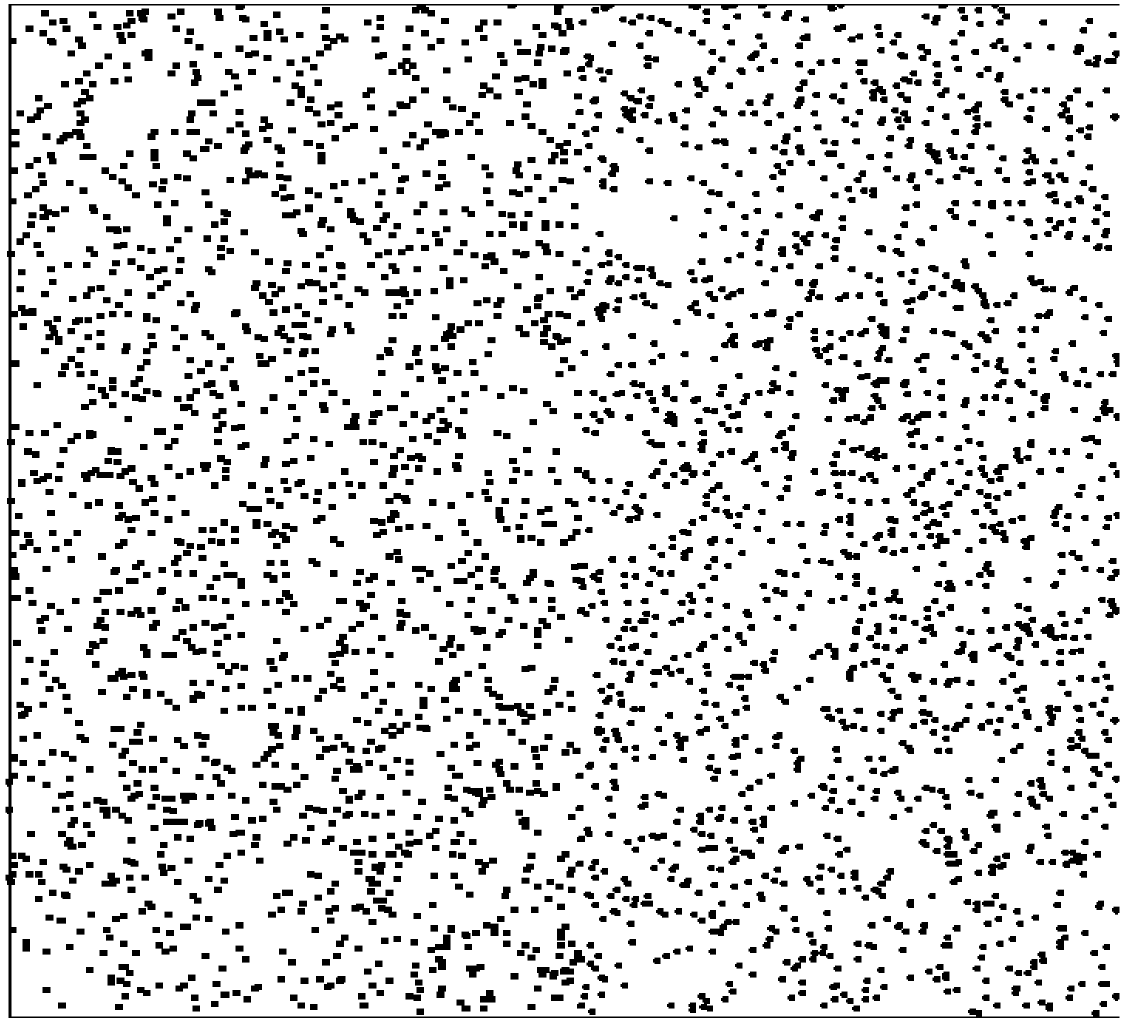
[Gabrielli, Jancovici, Joyce, Lebowitz, Pietronero and Labini, 2002]



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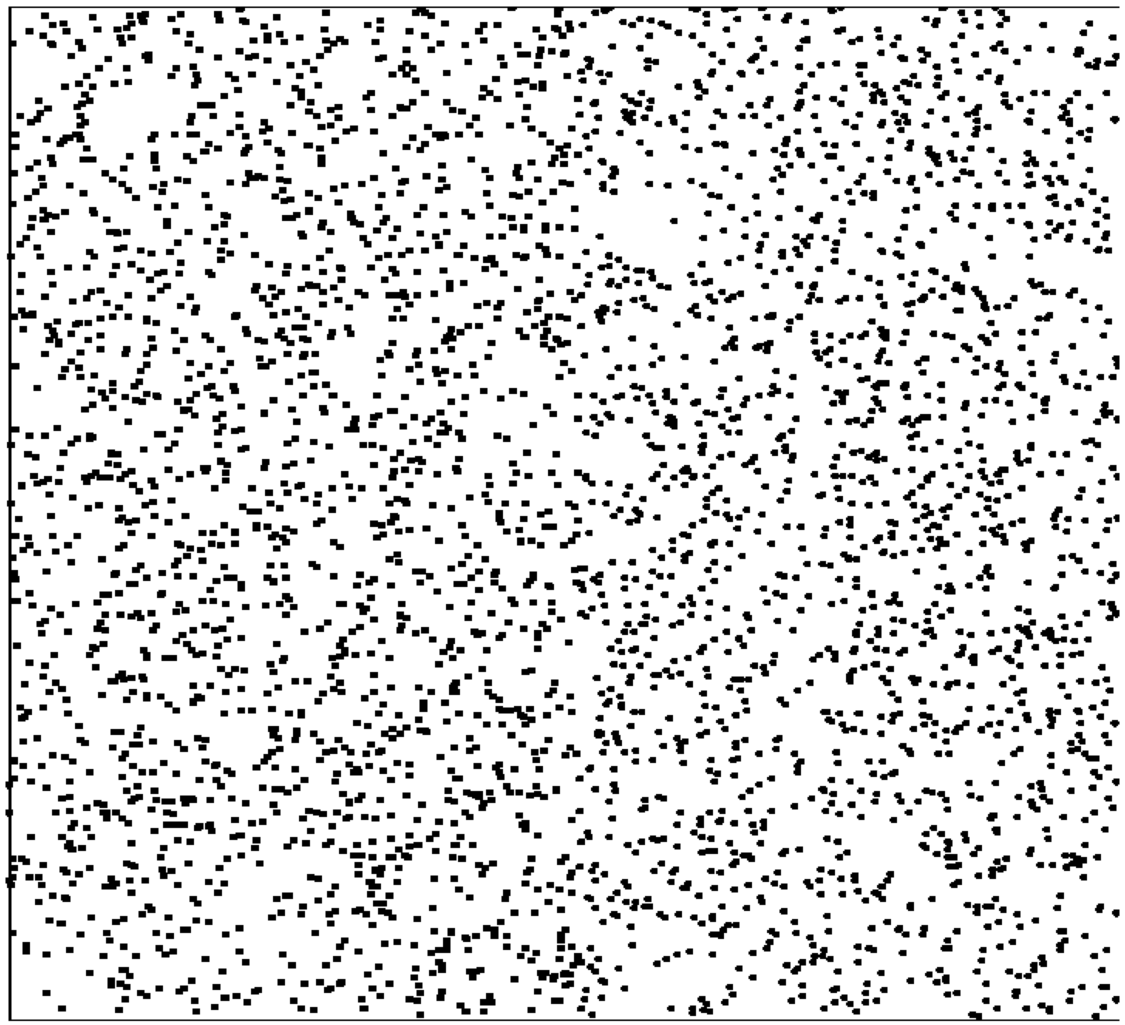

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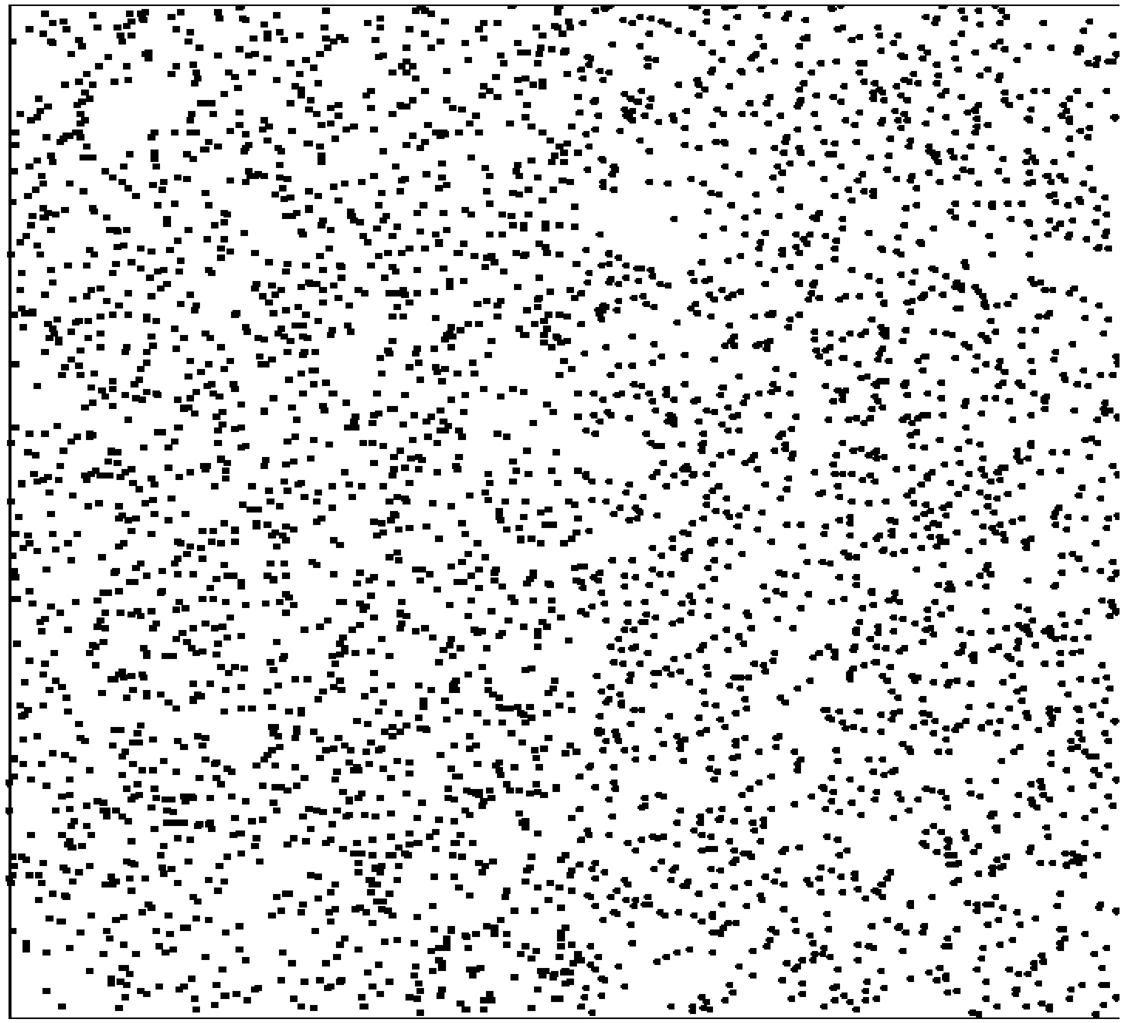

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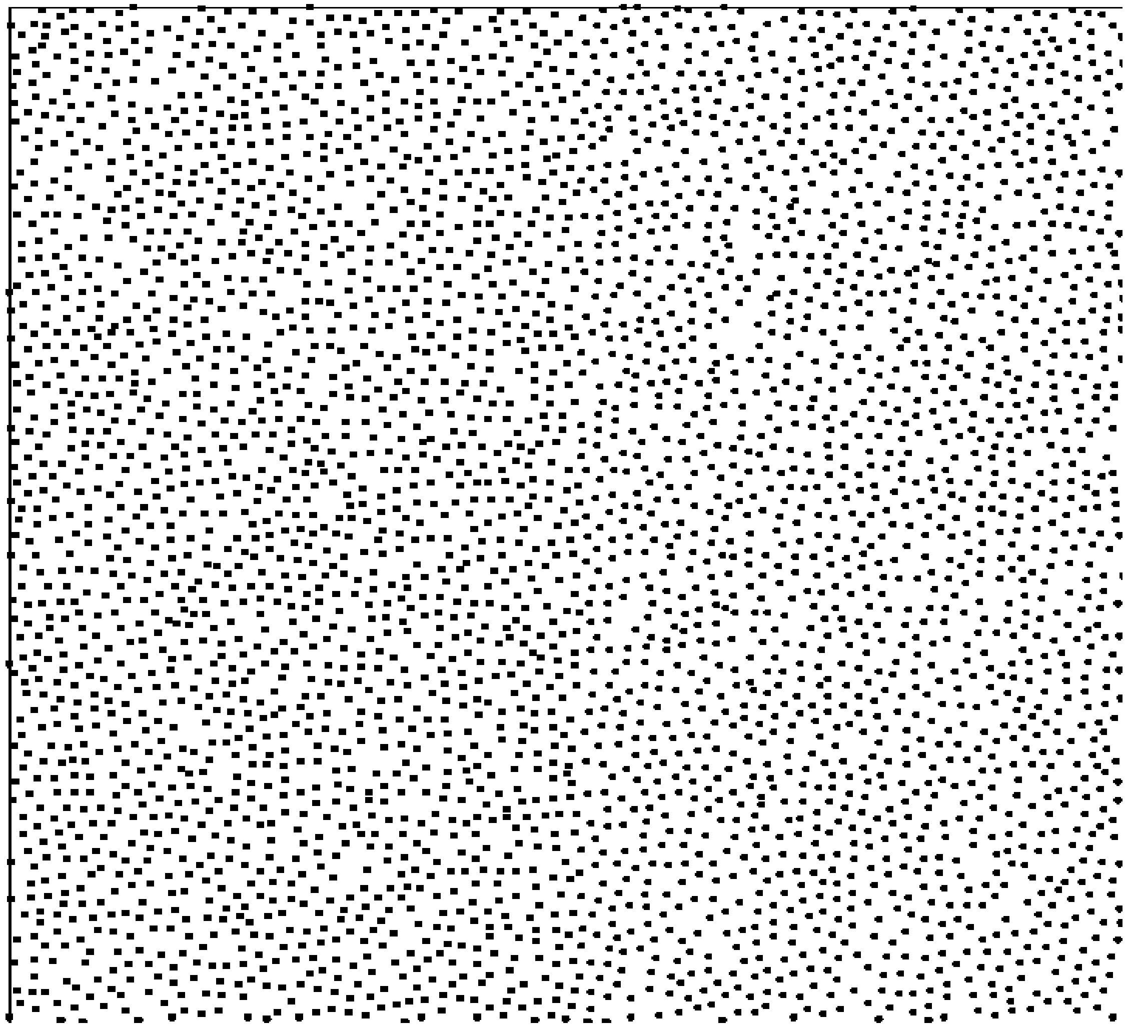

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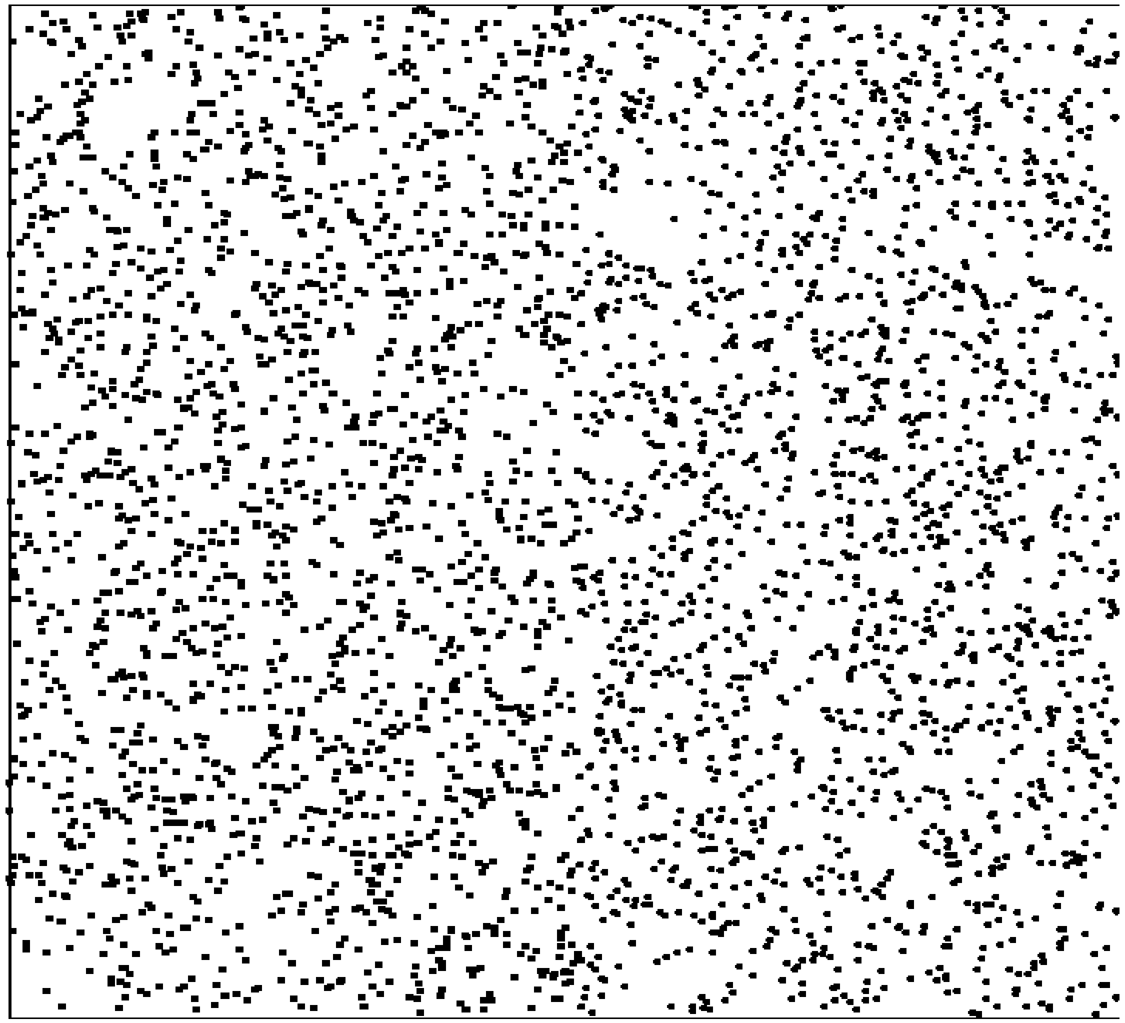

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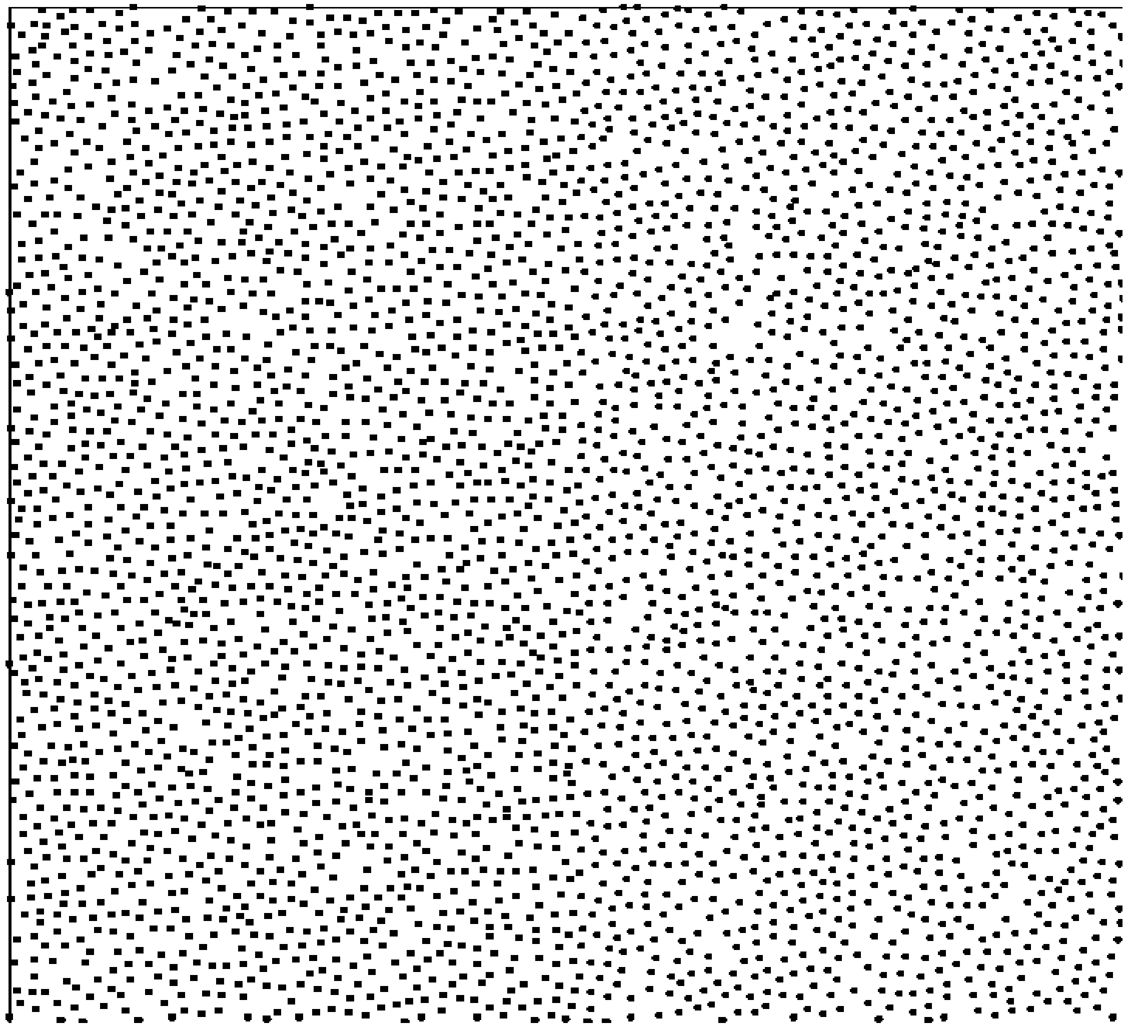

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For extreme bias, can get exact results (Bethe ansatz):

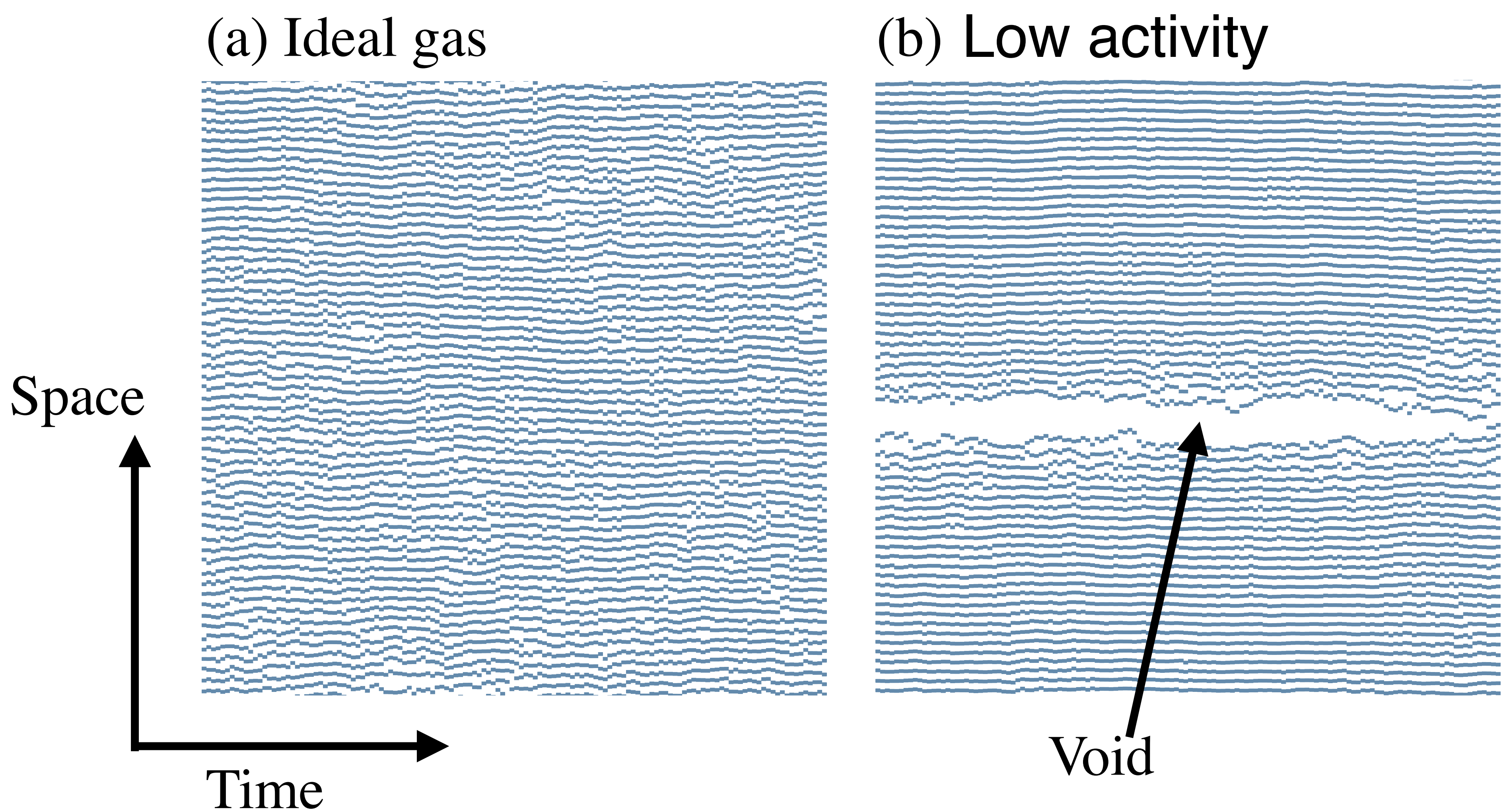
[Schuetz, Simon, Popkov, Lazarescu, 2009-]

Repulsive potential $V(i-j) \sim -\log \sin \frac{\pi(i-j)}{2L}$

That is, particles on a *circle* interact by ($2d$) Coulomb repulsion

“Phase separation”

Hard particles in 1d evolving with Brownian motion (Langevin), conditioned on low activity



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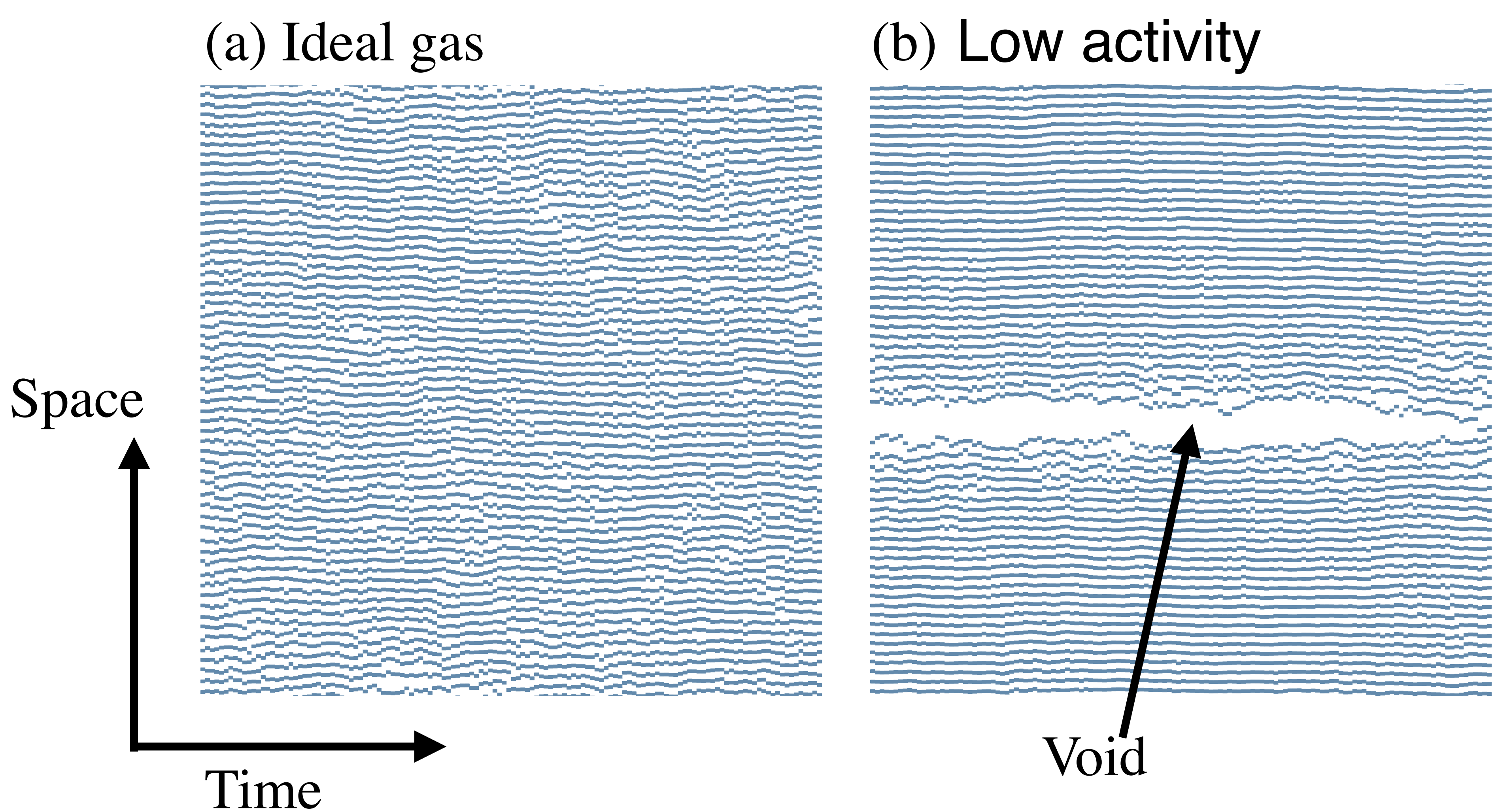

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Linear response

[RLJ, Thompson, Sollich, PRL **114,** 060601 (2015)]

General result: can obtain effective potential values from "propensities" for activity

$u(\mathcal{C}, s) \propto \langle \mathrm{e}^{-sK} \rangle_{\mathcal{C}(0)=\mathcal{C}}$

(average over long trajectories starting in $\mathcal{C}$, need to take care with normalisation)

Simple hydrodynamic argument shows that u-values for phase-separated / hyperuniform configurations have divergent $du(\mathcal{C}, s)/ds$ as system size $L \to \infty$.

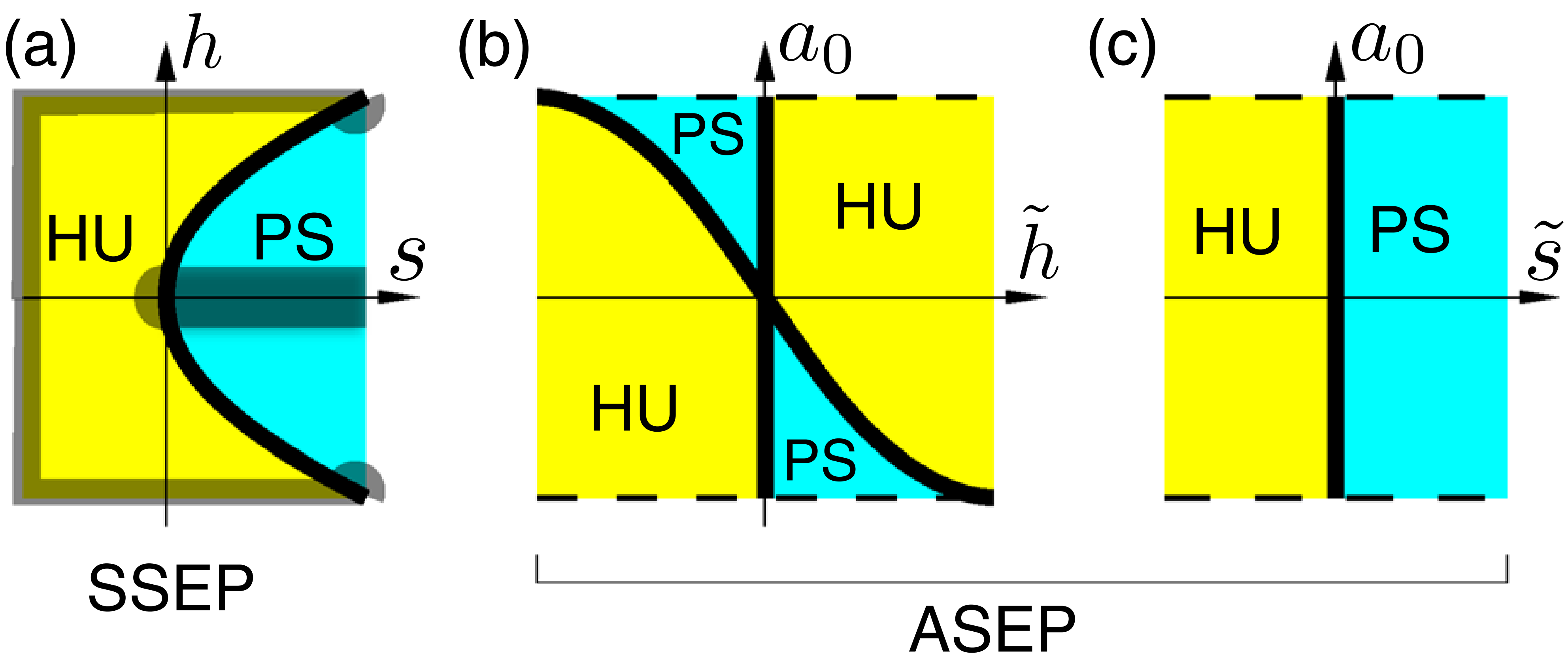
This comes from a diverging time scale: $\tau_L \sim L^2$ is the time required for these trajectories to relax to the steady state. . .

Diverging interaction range linked to diverging length and time scales. . .

Exclusion processes summary

[RLJ, Thompson, Sollich, PRL **114,** 060601 (2015)]

Long-ranged effective interactions (repulsive or attractive) are generic in conditioned exclusion processes



The physical origin of the weak-bias instabilities is the diverging hydrodynamic time scale $\tau_R \sim R^2$.

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Site i has occupancy $n_i \in \{0, 1\}$

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Simple model for glassy dynamics, stationary state has trivial product structure

[Jackle & Kronig 1991, Garrahan & Chandler, 2003-]

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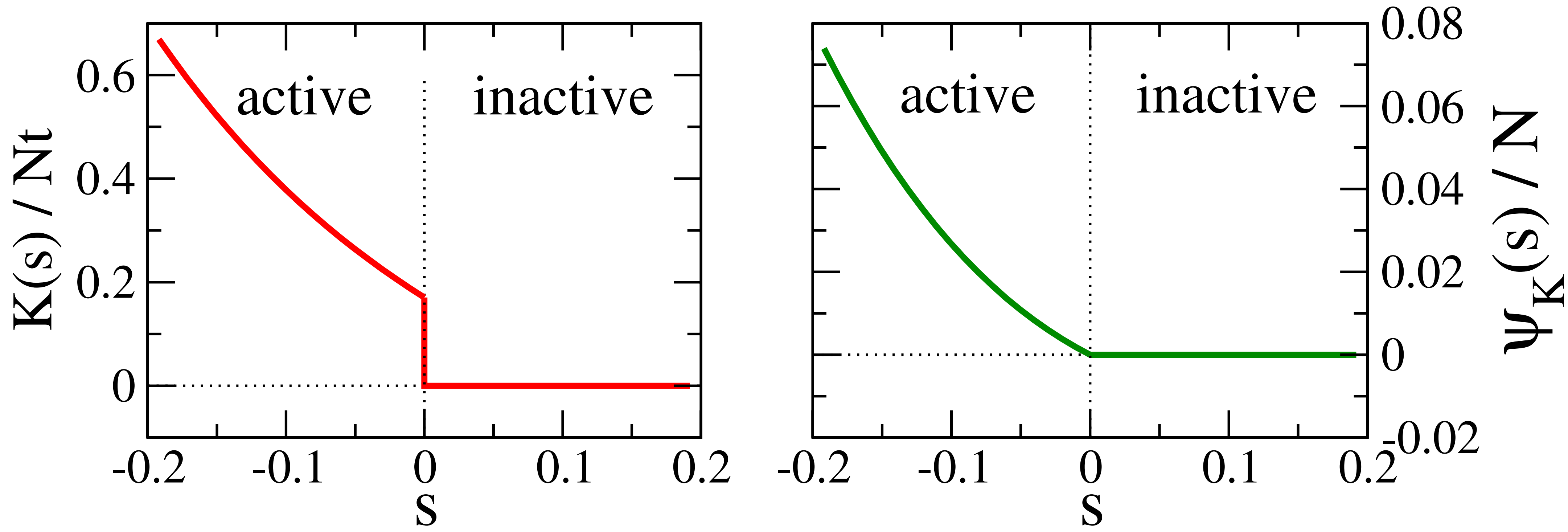
Relaxation time diverges for small c as

$$\log \tau \sim a(\log c)^2$$

Hierarchical relaxation mechanism…

[Sollich & Evans 1999, Aldous & Diaconis 2002, Toninelli, Martinelli & others 2007-]

East model : phase transition



$$K(s)/t = -\psi'(s)$$

As system size $N \to \infty$, there is a jump in the first derivative of the "free energy" $\psi(s)/N$.

First order dynamical phase transition, accompanied by *phase separation in space-time*

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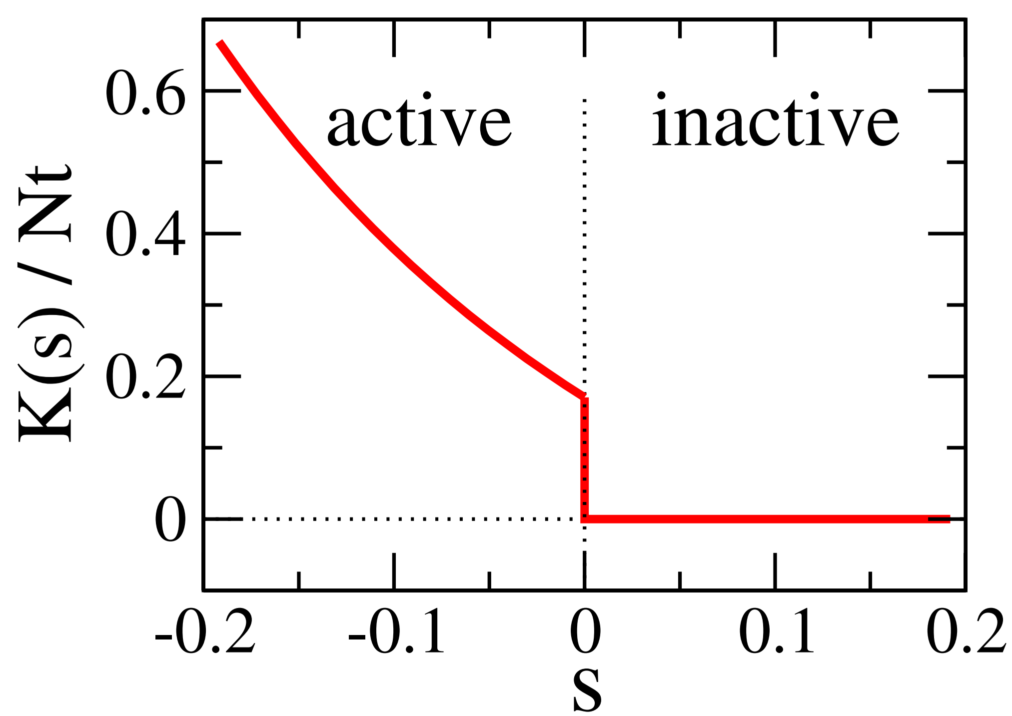

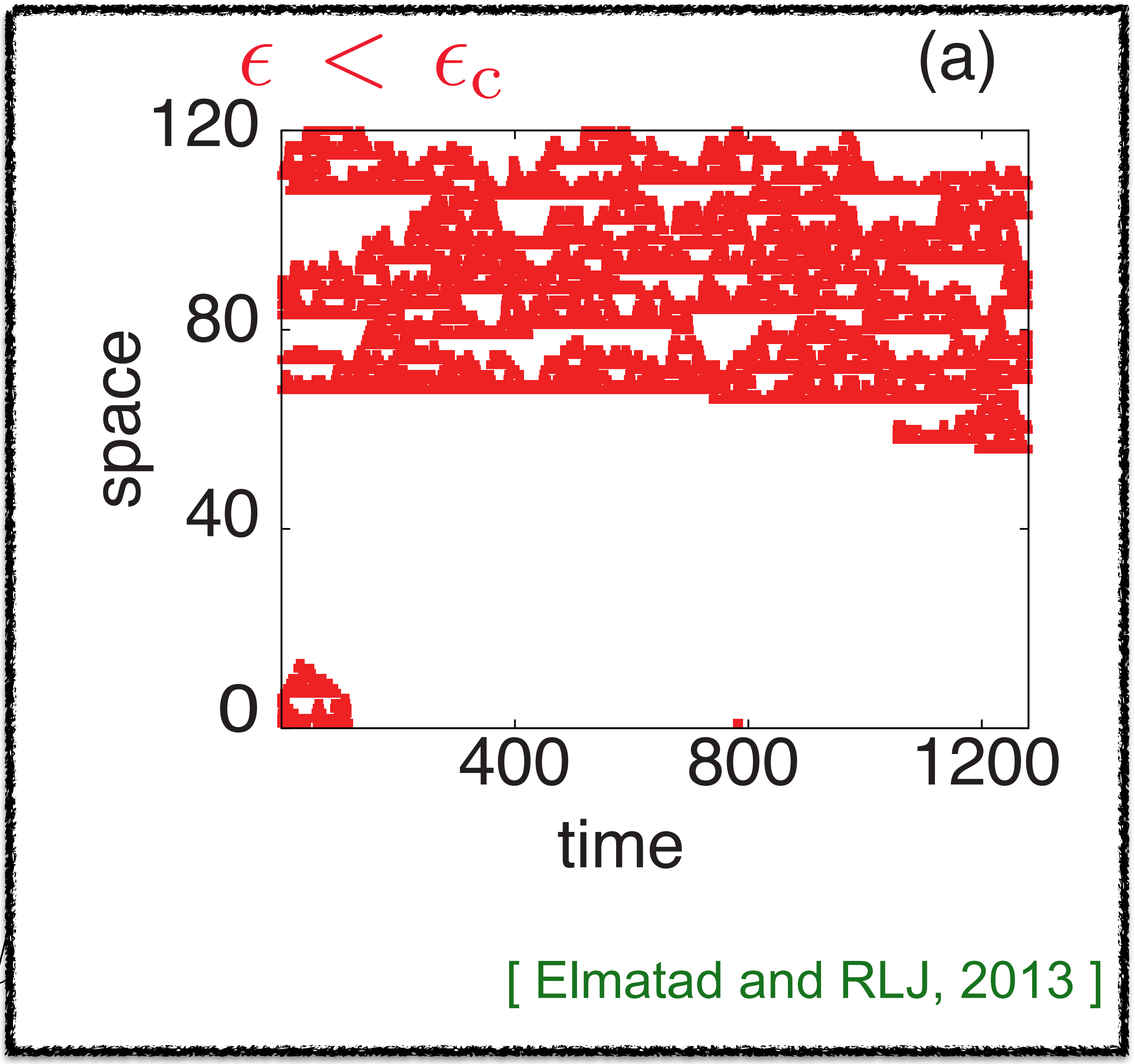

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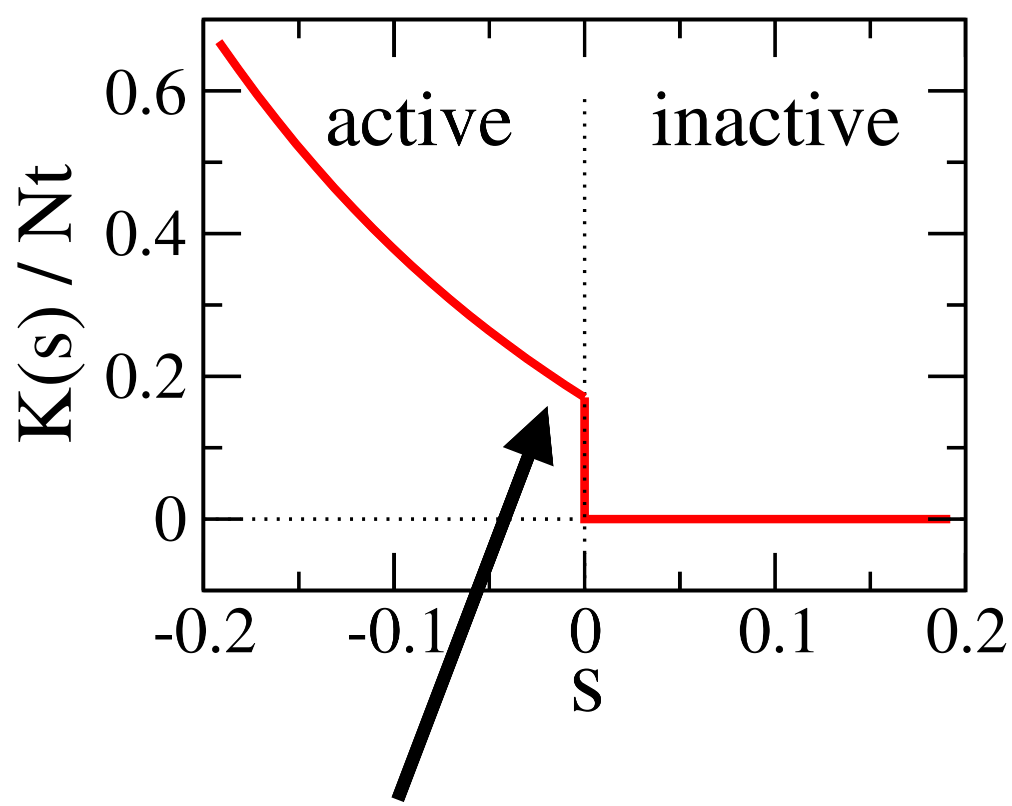
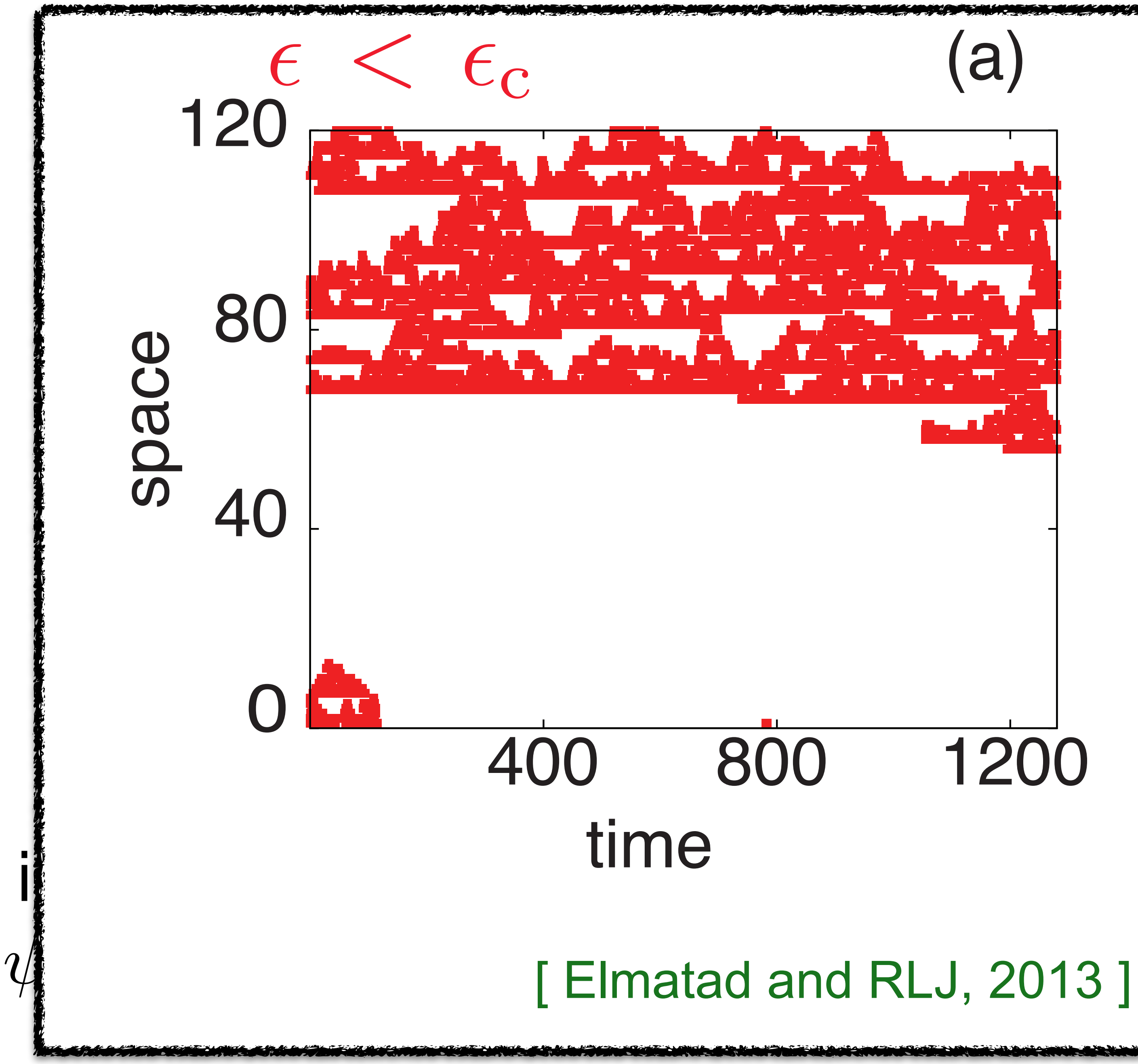


What happens here?



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Hence $u(\mathcal{C}) = \langle \mathcal{C}|\pi^{-1/2}|v^*\rangle$ where $|v^*\rangle$ is the maximiser

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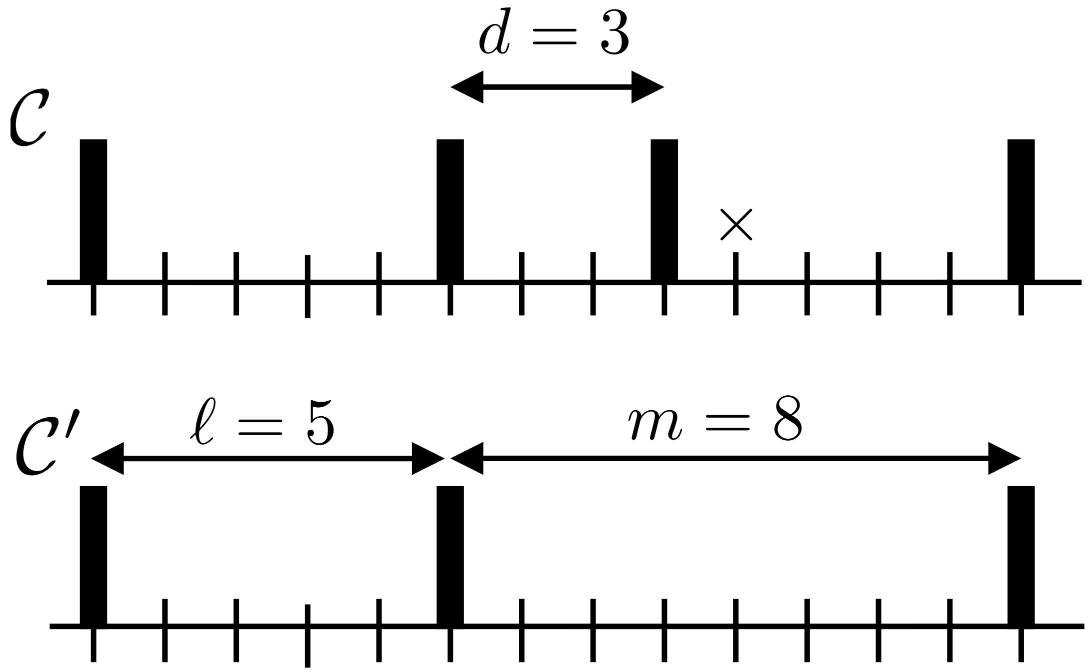
Hence $u(\mathcal{C}) = \langle\mathcal{C}|\pi^{-1/2}|v^*\rangle$ where $|v^*\rangle$ is the maximiser

(Variational problem with 2^N d.o.f.)

Conditioned East model

[RLJ and Sollich, J Phys A, 2014]

East model, biased to high activity



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Variational results using ansatze for *effective interactions*

1. local multi-spin interactions up to 6-body
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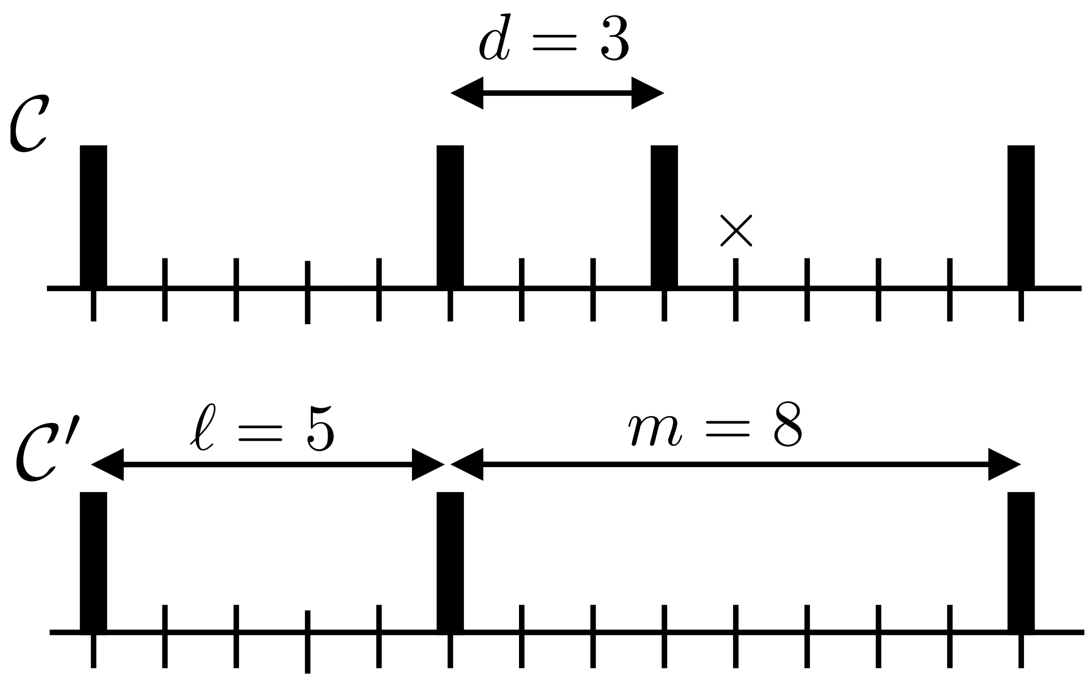

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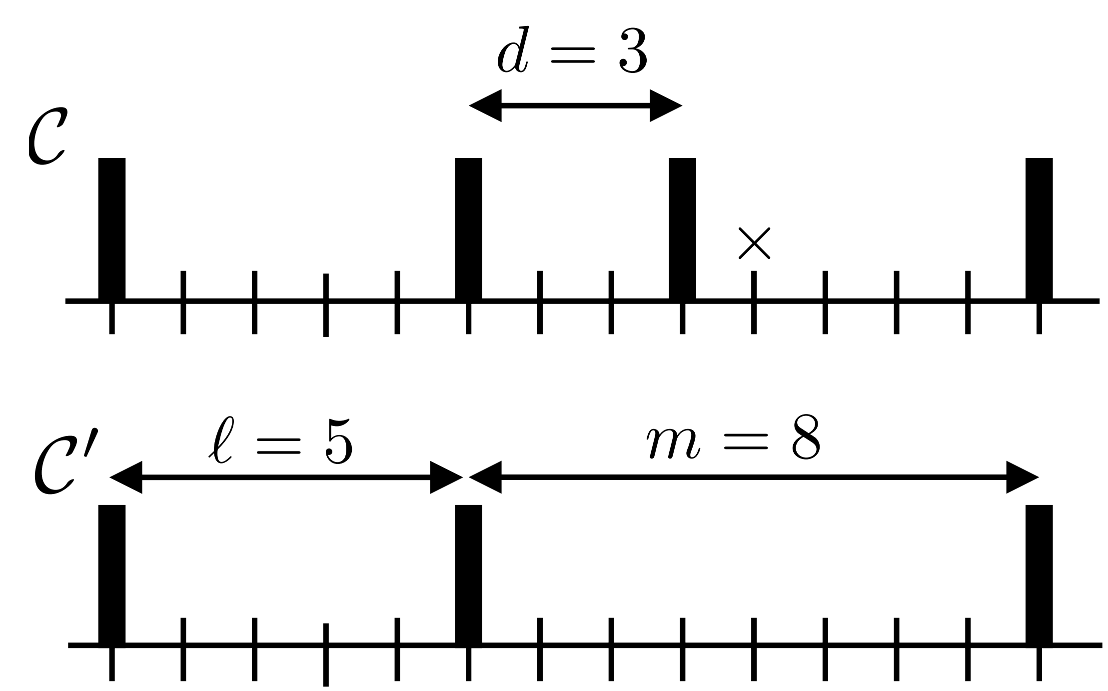
Also,
numerical results
(exact diagonalisation
 and transition path sampling)

… and perturbative results for small bias



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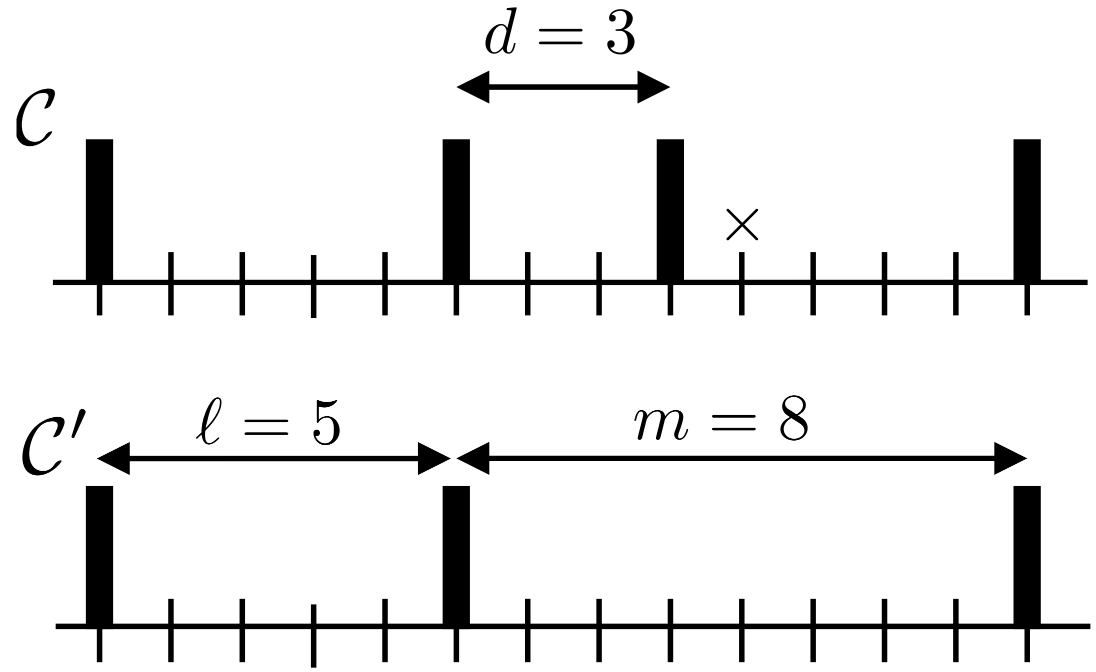
Main results:



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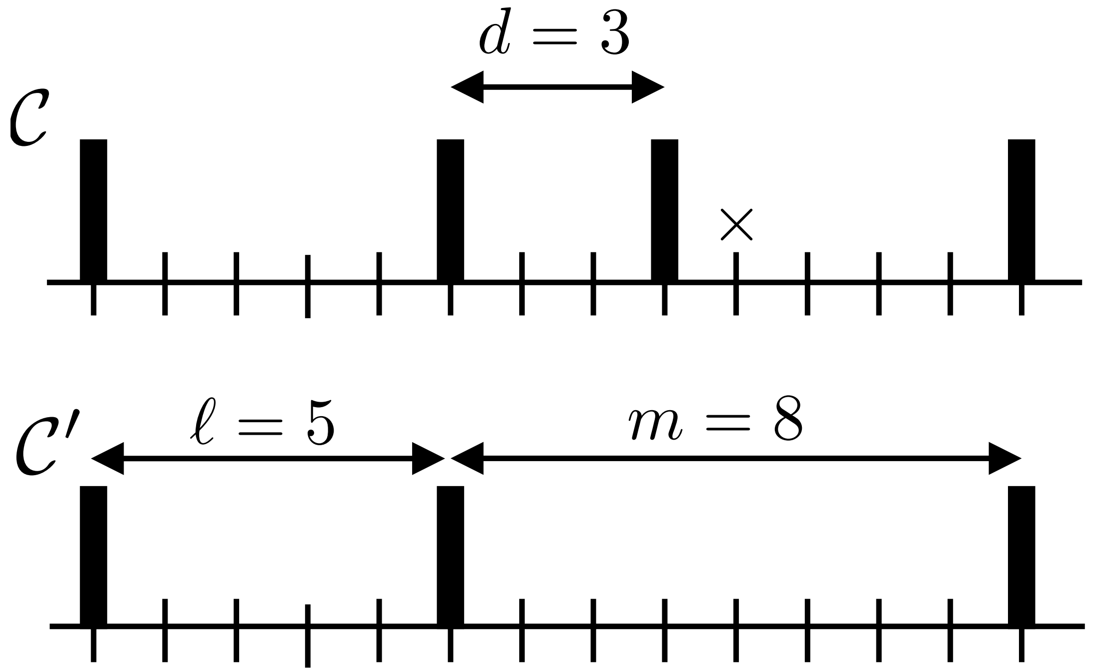
[RLJ and Sollich, J Phys A, 2014]

Main results:

Interactions are *long-ranged,* (no finite ranged interaction can capture even the first-order response to the bias)
can attribute this long range to large time scales for relaxation on large length scale (cf SEP)



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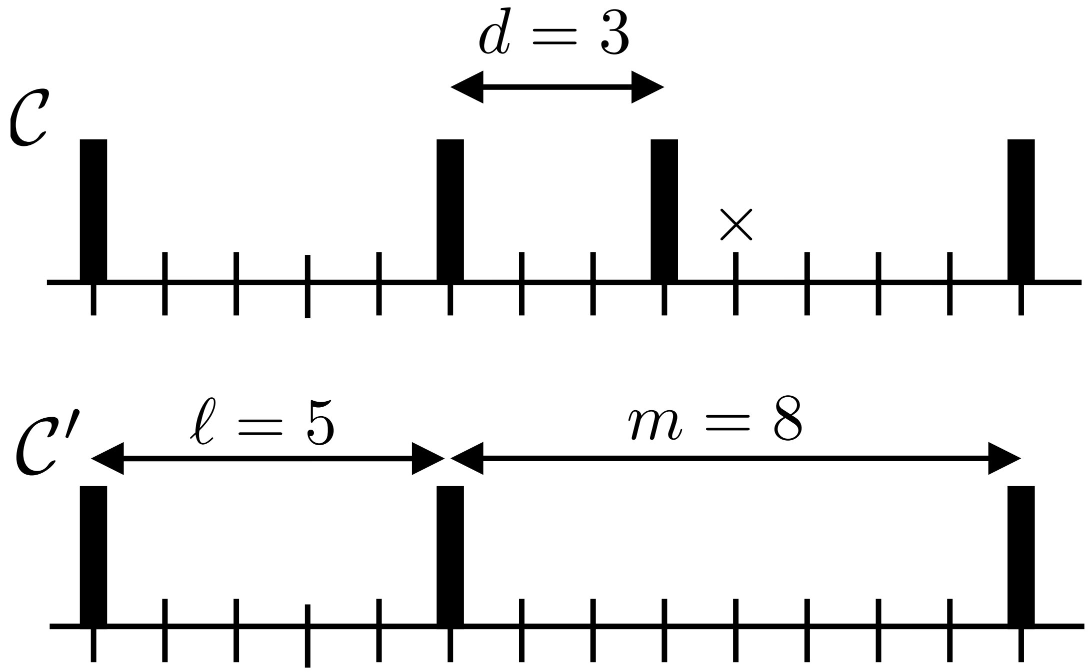

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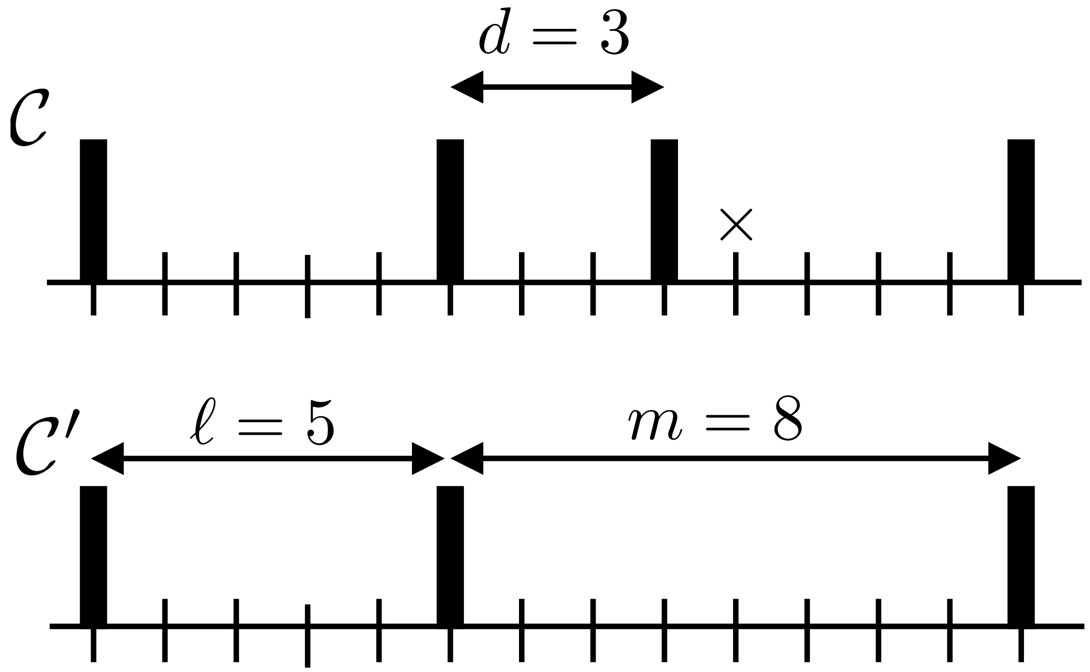

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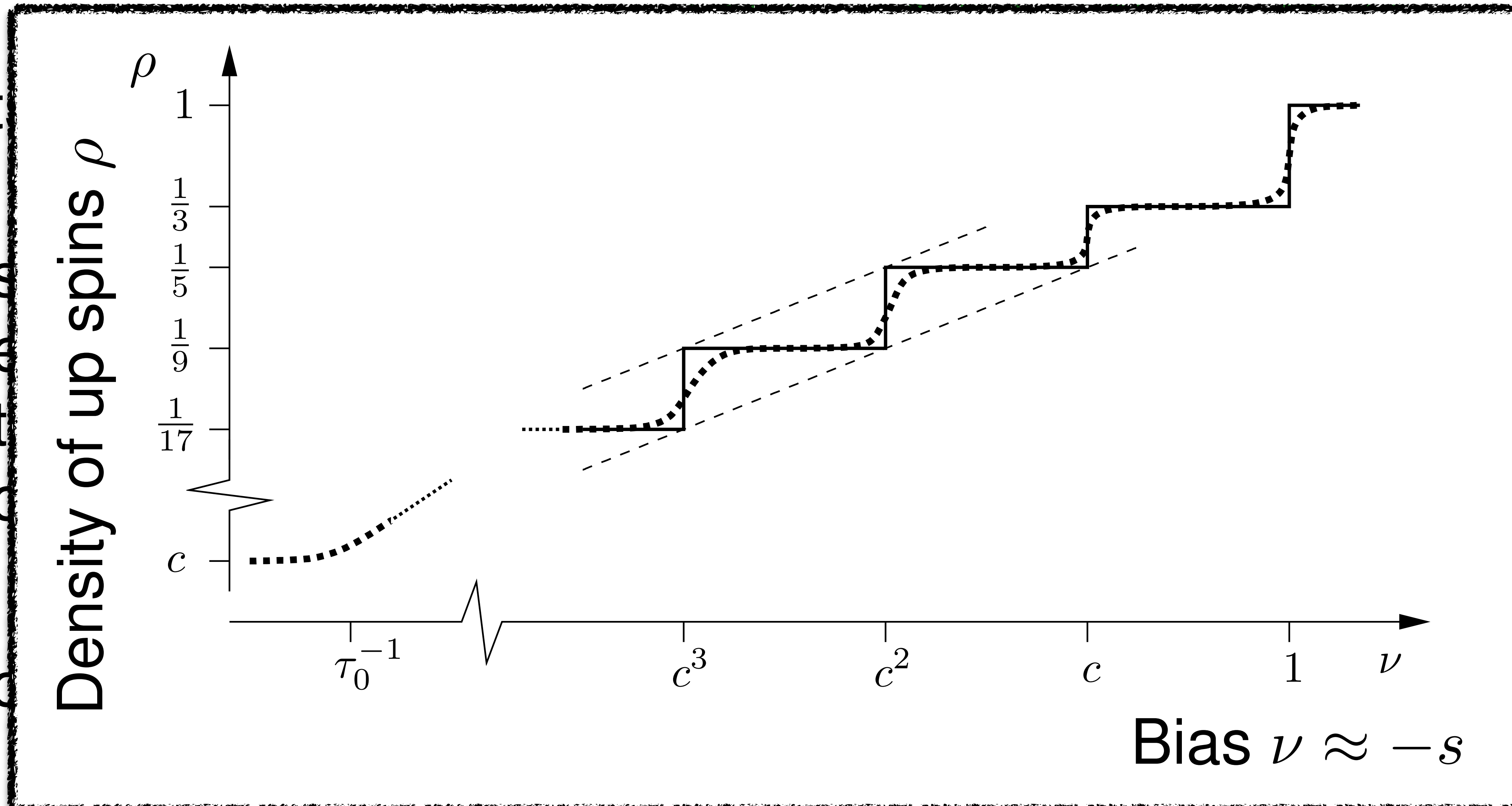

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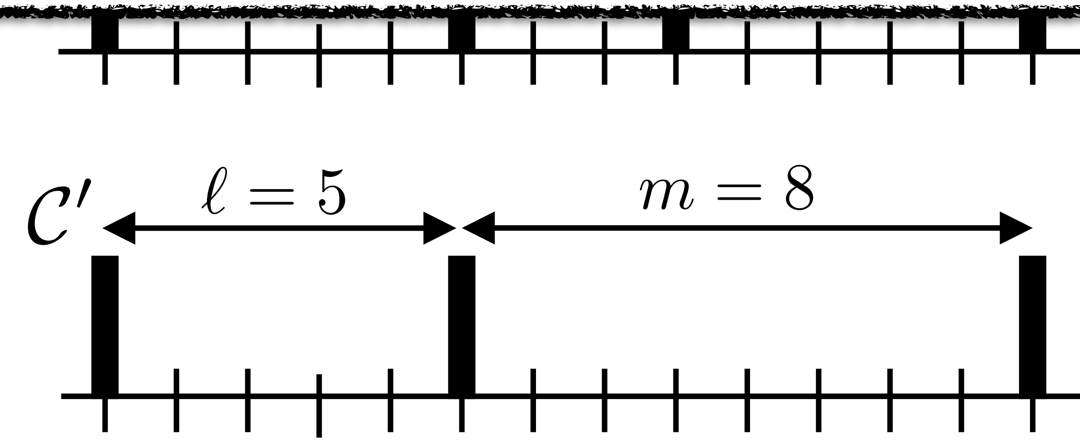

Summary so far

In East model and exclusion processes,
several things go together

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There are good reasons to expect this to be general:
(eg perturbative arguments, small spectral gaps…)
… also, plenty of other examples

1d Ising model

Consider $1d$ Glauber-Ising chain (periodic) conditioned on time-integrated energy

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(how general is this?)

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Conditioning stochastic systems to non-typical values of time-integrated observables leads to rich phenomenology

Hyperuniformity, phase separation in space and/or time, dynamical phase transitions, hierarchical responses…

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Long-ranged, non-Gibbsian, absence of dissipation

Slow degrees of freedom respond most strongly to bias (or conditioning), this can be one origin of long-ranged interactions

[more info: RLJ & Sollich, EPJE 2015, Touchette and Chetrite arXiv 1506.05291]