Effective dynamics and timescale separation in the East model

Alessandra Faggionato

University La Sapienza - Rome

P. Chleboun, F. Martinelli, C. Roberto, C. Toninelli

Motivations

Glasses are intriguing materials: mechanical rigidity similar to crystalline media, despite absence of long–range order.

Some key features of their evolution (common to other amorphous materials):

- **Extremely slow dynamics**
- **Dynamic heterogeneity**

Dynamic heterogeneity

- **supported by simulations and measurements of relaxation spectra;**
- **a very broad range of relaxation times with transient spatial fluctuations in local dynamics**

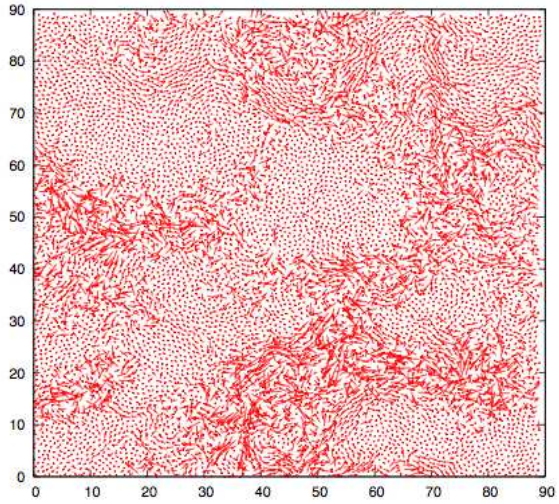


Figure: **Particle displacements in a 2D supercooled liquid. Physics 4, 42 (2011) L. Berthier**

East model

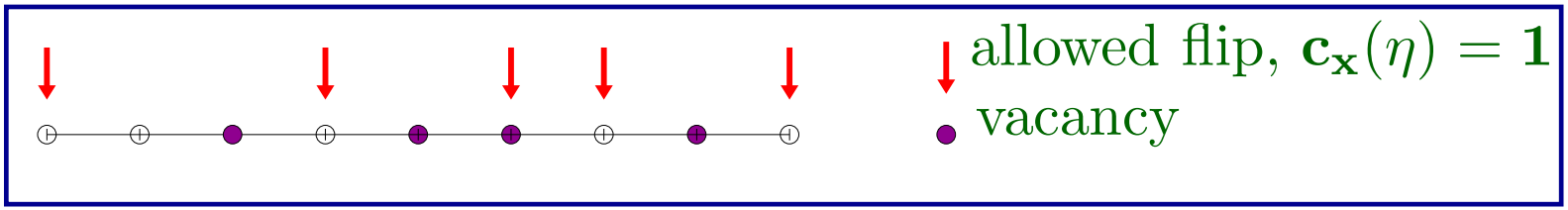
- $\mathbf{q} \in (\mathbf{0}, \mathbf{1})$ **parameter**
- **box** $[\mathbf{1}, \mathbf{L}] \subset \mathbb{N}$
- **configurations** $\eta \in \{\mathbf{0}, \mathbf{1}\}^{\mathbf{L}}$, $\eta_{\mathbf{x}} = \begin{cases} \mathbf{1} & \textbf{particle at x} \\ \mathbf{0} & \textbf{vacancy at x} \end{cases}$
- **Spin–flip dynamics**:
  - $\rightarrow$ **for each site x, wait at x an exponential time of mean 1**
  - $\rightarrow$ **afterwards, if** $\mathbf{c_x}(\eta) = \mathbf{1}$**, refresh** $\eta_{\mathbf{x}}$ **as** $\begin{cases} \mathbf{1} & \text{prob. } \mathbf{1} - \mathbf{q} \\ \mathbf{0} & \text{prob. } \mathbf{q} \end{cases}$

Dynamical constraint

Dynamical constraint at x:

$$\mathbf{c_x}(\eta) = \begin{cases} \mathbb{1}(\eta_{\mathbf{x-1}} = \mathbf{0}) & \text{if } \mathbf{2} \leq \mathbf{x} \leq \mathbf{L} \\ \mathbf{1} & \text{if } \mathbf{x} = \mathbf{1} \end{cases}$$

Site 1 behaves as with a frozen vacancy at 0



Waves of vacancies

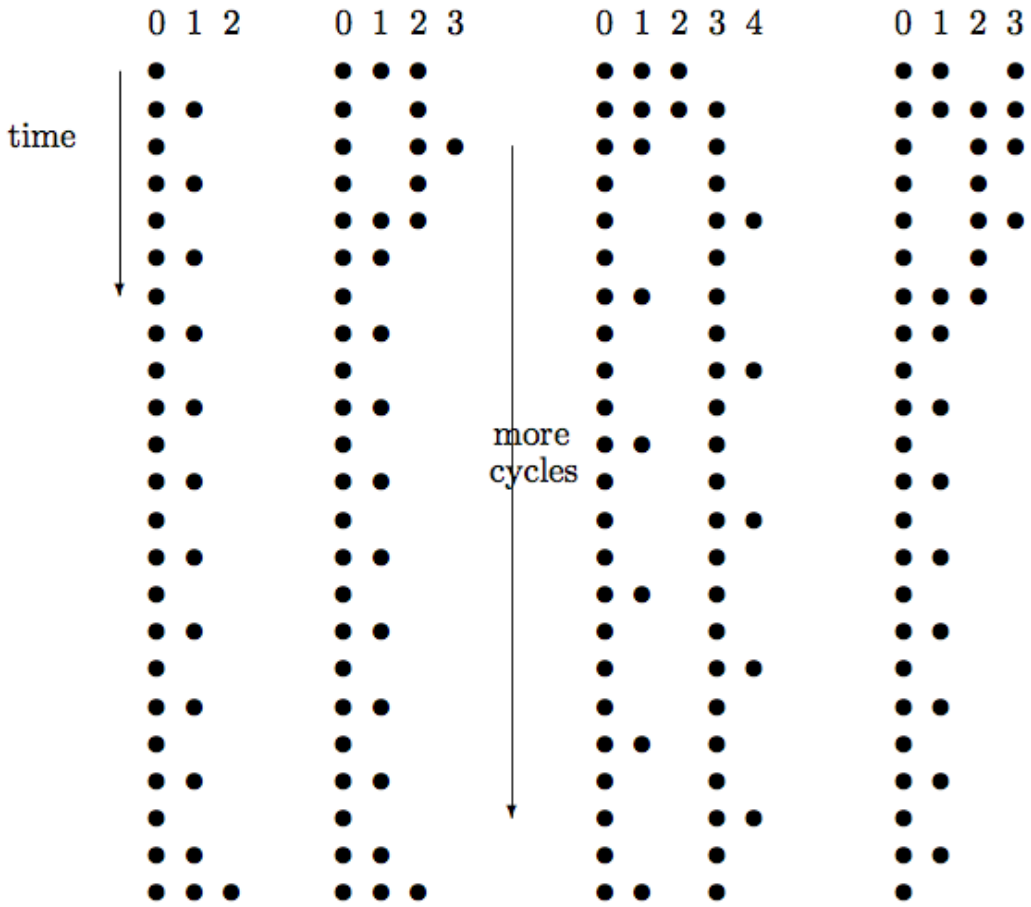


Figure: Source: Aldous, Diaconis JSP **107**

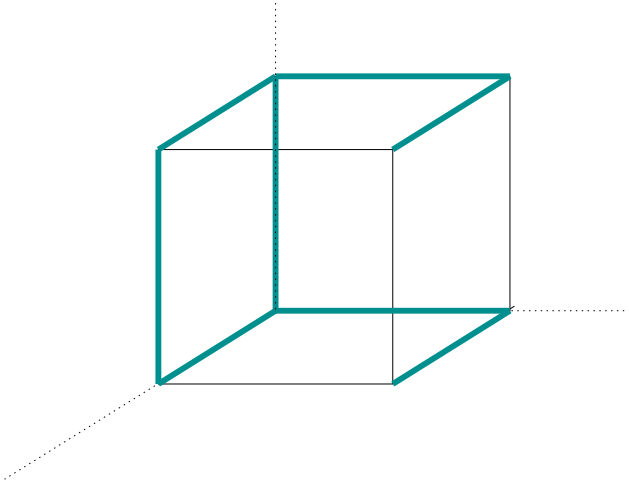
Energetic considerations

- $\mathbf{q} = \frac{\mathbf{e}^{-\beta}}{\mathbf{1}+\mathbf{e}^{-\beta}}$ β **inverse temperature**
- **interesting regime: low temperature,** $\mathbf{q} \downarrow \mathbf{0}$
- **Hamiltonian** $\mathbf{H}(\eta) = -\sum_{\mathbf{x}=\mathbf{1}}^{\mathbf{L}} \eta_{\mathbf{x}}$
  trivial energy landscape
- **Ground state: filled configuration** $\mathbb{1}$
- $\pi := (\mathbf{1}-\mathbf{q})$**–Bernoulli probability measure on** $\{\mathbf{0},\mathbf{1}\}^{\mathbf{L}}$
- π **reversible (detailed balance OK)**
- $\mathbf{1}/\mathbf{q} =$ **equilibrium mean distance consec. vacancies**

Random walk on subgraph of hypercube

- **State space $\{0,1\}^{\mathbf{L}}$, hypercube**
- **Random walk on subgraph $\mathcal{G}$ of hypercube**
- **vertexes $\mathcal{G}$ = vertexes of hypercube**
- **edges $\mathcal{G} \subset$ edges of hypercube**

Figure: **Subgraph $\mathcal{G}$, $\mathbf{L} = 3$**



Allowed jumps

Complex underlying graph $\mathcal{G}$

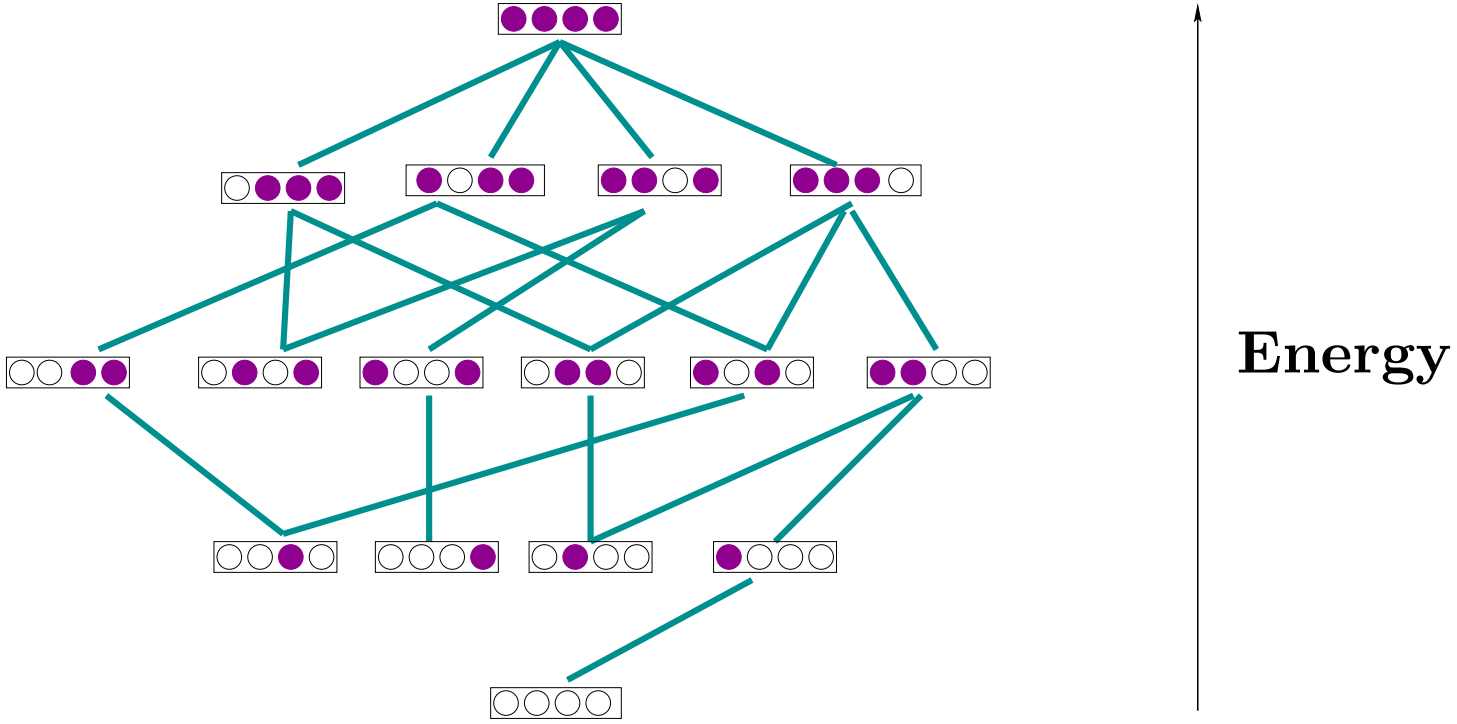
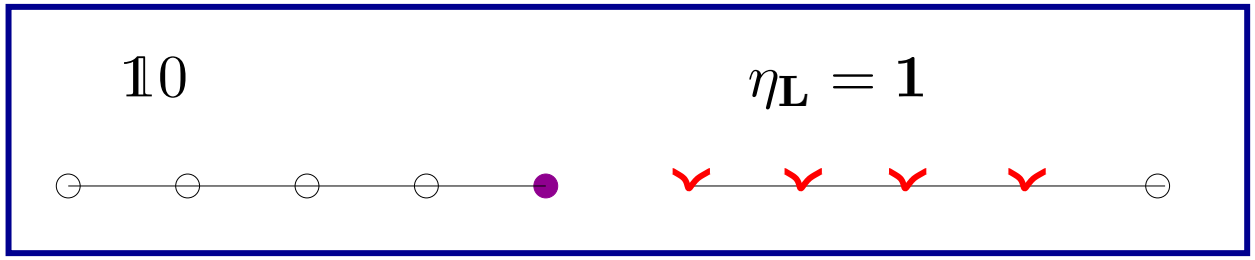


Figure: **Underlying graph for East dynamics, L = 4**

Characteristic times

- **Relaxation time**: $\mathbf{T_{rel}(L) = 1/gap(\mathcal{L}^{(L)})}$
- **Mixing time**:
  $\mathbf{T_{mix}(L)} = \inf_{\mathbf{t \geq 0}} \left\{ \|\mathbf{P_t}(\eta, \cdot) - \pi\|_{\mathbf{TV}} \leq \mathbf{1/4}\,, \forall \eta \right\}$
- **Hitting time**: $\mathbb{E}_{\mathbb{1}0}\left[\tau_{\eta_{\mathbf{L}}=\mathbf{1}}\right]$



All characteristic times are increasing in L

Equivalence of characteristic times

Theorem

- **If** $\mathbf{L = L(q) \leq d/q}$, **then** $\mathbf{T_{rel}(L)}$, $\mathbf{T_{mix}(L)}$ **and** $\mathbb{E}_{\mathbb{1}0}\left[\tau_{\eta_{\mathbf{L}}=\mathbf{1}}\right]$ **are equivalent**:

$$\mathbf{T_{mix}(L)/T_{rel}(L)} \quad , \quad \mathbb{E}_{\mathbb{1}0}\left[\tau_{\eta_{\mathbf{L}}=\mathbf{1}}\right]/\mathbf{T_{rel}(L)} \in \left[\mathbf{c(d)}, \mathbf{c'(d)}\right].$$

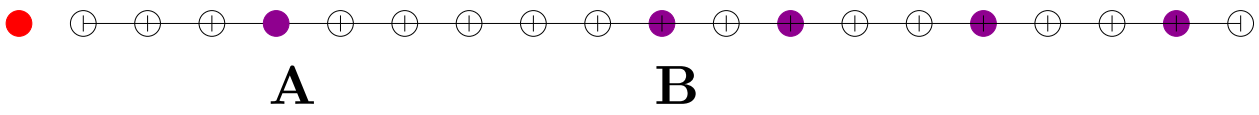
- **If** $\lim_{\mathbf{q}\downarrow\mathbf{0}} \mathbf{qL(q) = 0}$, **then**

$$\mathbf{T_{mix}(L)/T_{rel}(L)} \quad , \quad \mathbb{E}_{\mathbb{1}0}\left[\tau_{\eta_{\mathbf{L}}=\mathbf{1}}\right]/\mathbf{T_{rel}(L)} \to \mathbf{1}.$$

Hitting time $\mathbb{E}_{\mathbb{1}0}\left[\tau_{\eta_{\mathbf{L}}=\mathbf{1}}\right]$

"Mixing times are hitting times of large sets" Peres, Sousi
In our case: large set $\{\eta_{\mathbf{L}} = \mathbf{1}\}$

Take a generic initial configuration



- **Until an initial vacancy is not removed, it behaves as the frozen vacancy at 0**
- **It creates waves of vacancies**
- **Interested in the time a wave created by A kills the vacancy at B**

Estimates of characteristic times

Theorem

Let $\mathbf{n} := \lceil \log_2 \mathbf{L} \rceil$, i.e. $2^{n-1} < L \leq 2^n$

- $L = \text{const.} \Rightarrow c(n)\frac{1}{q^n} \leq T_{\text{rel}}(L) \leq c'(n)\frac{1}{q^n}$
- $L \leq d/q \Rightarrow \frac{n!}{q^n 2^{\binom{n}{2}}} q^{\alpha} \leq T_{\text{rel}}(L) \leq \frac{n!}{q^n 2^{\binom{n}{2}}} q^{-\alpha'}$

  where α, α' depend on d

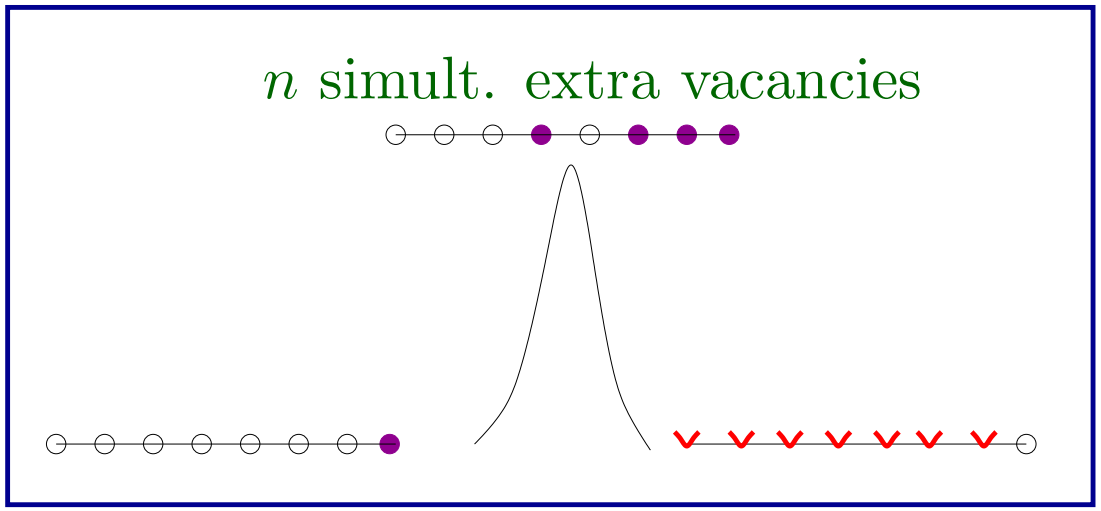
$$L = 1/q^{\gamma},\ \gamma \in (0,1] \ \Rightarrow\ \frac{n!}{q^n 2^{\binom{n}{2}}} \sim \frac{1}{q^{(1-\frac{\gamma}{2})n + \gamma \log_2 n}}\ , \quad n = \log_2 \frac{1}{q^{\gamma}}$$

Fact (CMRT)

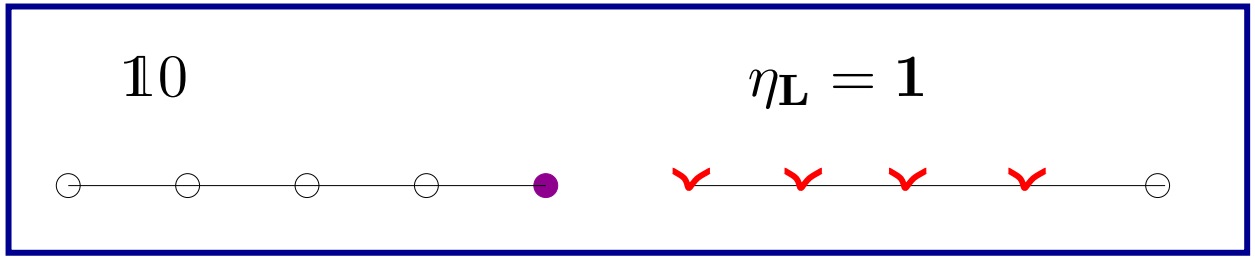
$\forall \delta > 0\ \exists C_{\delta} > 0$ s.t. $\forall L\ T_{\text{rel}}(L) \leq C_{\delta} \frac{1}{q^{\frac{n}{2-\delta}}}$, ; $\quad n = \log_2 \frac{1}{q}$

Minimal energy barrier

[CDG] if $2^{n-1} < L \leq 2^n$, i.e. $n = \lceil \log_2 n \rceil$, then



Energy and entropy



- $\mathbf{L} = \mathbf{const} \Rightarrow \mathbf{T_{rel}(L)} \sim \mathbf{(1/q)^n}$
  Up to $\tau_{\eta_{\mathbf{L}}=\mathbf{1}}$, max. n simultaneous extra vacancies
- **Case $\mathbf{L} = \mathbf{d/q^{\gamma}}$, $\gamma \in (\mathbf{0}, \mathbf{1}]$**
  1. $\mathbf{T_{rel}(L)} \ll \mathbf{(1/q)^n}$
  2. **Entropic corrections**
  3. **Up to $\tau_{\eta_{\mathbf{L}}=\mathbf{1}}$, max. $n+k$ simultaneous extra vacancies**

Timescale separation

Given $\mathbf{L'(q) \geq L(q)}$ we write

$$\mathbf{T_{rel}\big(L'(q)\big) \succ T_{rel}\big(L(q)\big)}$$

and say there is timescale separation between $\mathbf{L'(q), L(q)}$ if $\exists \beta > \mathbf{0}$ such that

$$\mathbf{T_{rel}(L'(q)) \geq q^{-\beta} T_{rel}(L(q))}$$

Timescale separation $\Rightarrow$ Dynamical heterogeneity
At time $\mathbf{T_{rel}(L(q))}$:

- **full evolution inside initial domains of length $\mathbf{L(q)}$**
- **partial evolution inside initial domains of length $\mathbf{L'(q)}$**

Corollary

- **Finite volume**
  Take $\mathbf{L', L}$ constant. Then

$$\mathbf{T_{rel}(L') \succ T_{rel}(L)}$$

  iff $\lceil \log_2 \mathbf{L'} \rceil > \lceil \log_2 \mathbf{L} \rceil$

- **Mesoscopic volume**
  Take $\mathbf{L(q) = d/q^{\gamma}}$ $\gamma \in (0,1)$. Then $\exists \mathbf{C = C}(\gamma) > 1$ s.t.

$$\mathbf{T_{rel}\big(CL(q)\big) \succ T_{rel}\big(L(q)\big)}$$

  If γ small $\Rightarrow \mathbf{C = 2}$

Continuous timescale separation hypothesis [ES]

Evans, Sollich
[Phys. Rev. Lett. 83 (1999). Phys. Rev. E **68** (2003)]

Conjecture (ES)

$\mathbf{T_{rel}}\left(\frac{\mathbf{d'}}{\mathbf{q}}\right) \succ \mathbf{T_{rel}}\left(\frac{\mathbf{d}}{\mathbf{q}}\right)$ **for all** $\mathbf{d' > d}$
More precisely

$$\mathbf{T_{rel}}\left(\frac{\mathbf{d}}{\mathbf{q}}\right) = \left(\frac{\mathbf{1}}{\mathbf{q}}\right)^{\mathbf{f(d)+o(1)}} \mathbf{T_{rel}}\left(\frac{\mathbf{1}}{\mathbf{q}}\right)$$

with $\mathbf{f}$ **strictly increasing**

The ES hypothesis is:

1. **supported by simulations**
2. **at the base of the "superdomain dynamics", effective dynamics near to equilibration**

Failure of the ES hypothesis

Theorem

- **The ES hypothesis fails:**

$$\mathbf{T_{rel}}\left(\frac{\mathbf{d}}{\mathbf{q}}\right) = \left(\frac{\mathbf{1}}{\mathbf{q}}\right)^{\mathbf{f(d)+o(1)}} \mathbf{T_{rel}}\left(\frac{\mathbf{1}}{\mathbf{q}}\right); \quad \mathbf{f \equiv 0}$$

- **No timescale separation between $\mathbf{d/q}$ and $\mathbf{d'/q}$**

What do simulations refer to?

- **Timescale separation at level $\mathbf{O(1/q^{\gamma})}$, $\gamma \in (\mathbf{0}, \mathbf{1})$**
- **Not clear nature:**

$$\begin{cases} \text{continuous} \\ \text{discrete} \end{cases} \qquad \mathbf{T_{rel}}\left(\frac{\mathbf{d'}}{\mathbf{q^{\gamma}}}\right) \succ \mathbf{T_{rel}}\left(\frac{\mathbf{d}}{\mathbf{q^{\gamma}}}\right); \qquad \mathbf{d' > d},$$

Effective dynamics: some basic observations

Effective dynamics: **Approximating dynamics, simpler, with less degrees of freedom, allowing predictions and better comprehension of the fundamental features of the original dynamics**

Regime $\mathbf{qL(q) \downarrow 0}$

(i) $\mathbf{P}\big(\textbf{vacancies } \eta(\mathbf{s}) \supset \textbf{vacancies } \eta(\mathbf{t})\big) = \mathbf{1} - \mathbf{o}(\mathbf{1}), \ \mathbf{s} < \mathbf{t}$

(ii) $\pi(\mathbb{1}) = \mathbf{1} - \mathbf{o}(\mathbf{1})$, $\mathbb{1}$ **filled configuration**

$\Rightarrow$ **Annihilation effective dynamics**

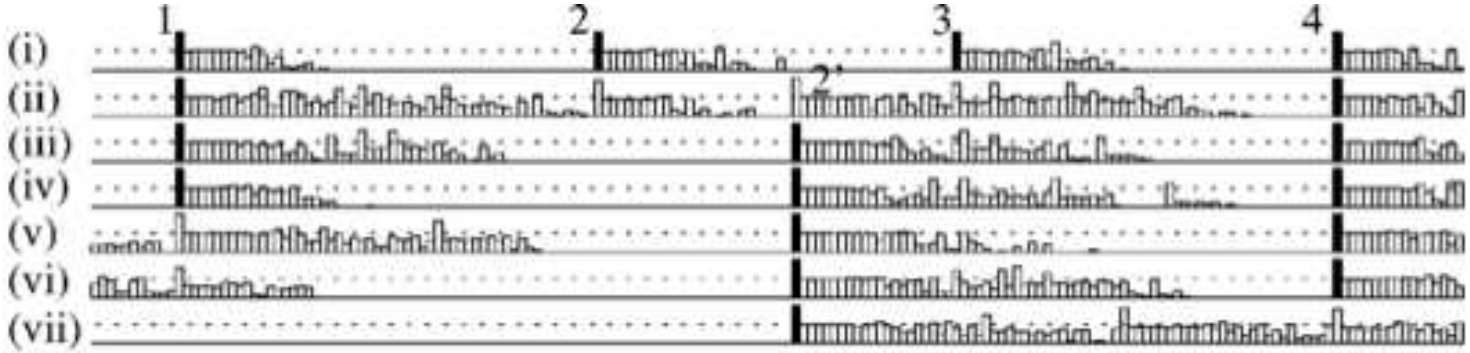
Regime $\mathbf{qL(q) \to d}$

$\Rightarrow$ **No annihilation effective dynamics**

Equilibrium effective dynamics

- $\mathbf{L \sim \Delta/q,\ \Delta \gg 1}$
- $\mathbf{t \geq T_{\,\mathrm{rel}}(1/q)}$

Evans, Sollich: superdomains dynamics



Based on the continuous timescale separation hypothesis

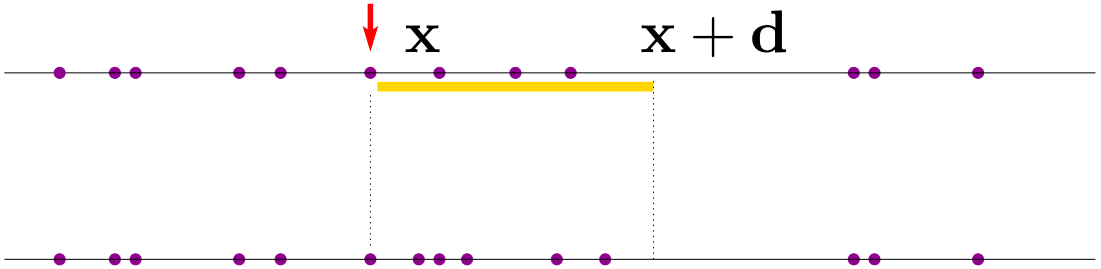
Aldous–Diaconis equilibrium effective dynamics

- **East process on** $\mathbb{N} = \{1, 2, \dots\}$
- **Map** $\eta_t \in \{0,1\}^{\mathbb{N}}$ **to** $\xi_t = \{x \in \mathbb{N} : \eta_x = 0\}$

Conjecture:

- $\left\{q\xi_{tT_{rel}(1/q)}\right\}_{t\geq 0} \to \{\Theta_t\}_{t\geq 0}$
- Θ_t **Poisson point process rate 1**
- **Each point creates "wave" of length** $> d$ **with rate** $G(d)$
- **The wave** $(x, x+d]$ **deletes points in** $(x, x+d]$ **and replace them by a Poisson point process rate 1**

The wave $(x, x+d]$ deletes points in $(x, x+d]$ and replace them by a Poisson point process rate 1

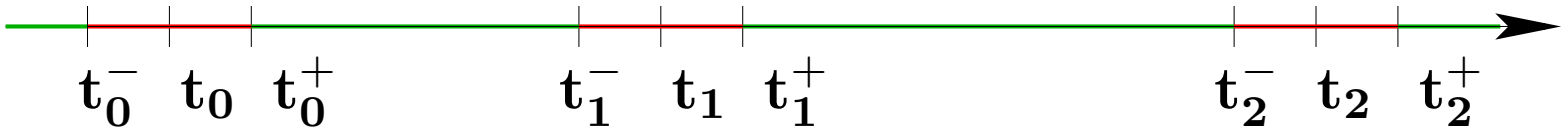


Effective dynamics for finite volume observations

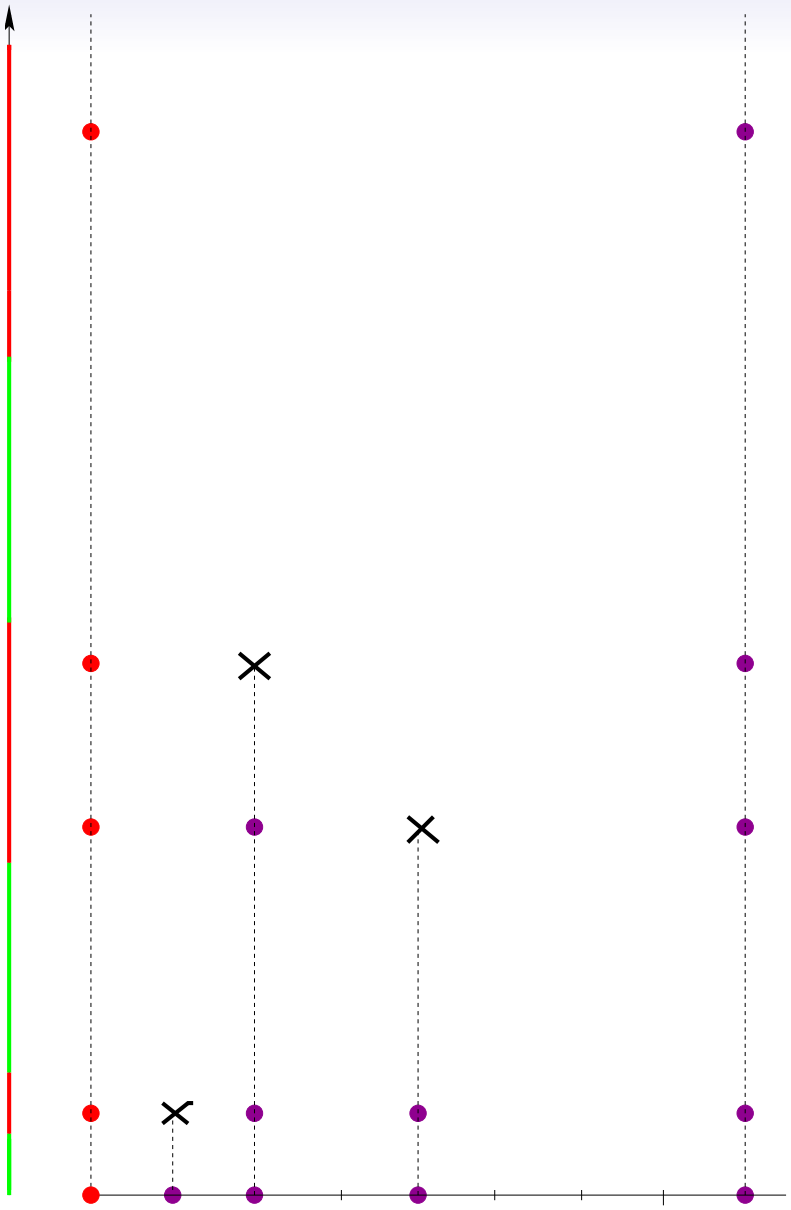
Complete analysis:
[ES, F.-Martinelli-Roberto-Toninelli CMP 309 (2012)]

Recall: $\mathbf{T_{rel}(L) = q^{-n}}$ **if** $\mathbf{n} = \lceil \log_2 \mathbf{L} \rceil$

Set $\mathbf{t_n = q^{-n}}$, $\mathbf{n = 0, 1, 2, \ldots}$



1. **In stalling periods no evolution**
2. **In active period** $[t_n^-, t_n^+]$ **coalescence dynamics, domains of length L s.t.** $\mathbf{n} = \lceil \log_2 \mathbf{L} \rceil$ **coalesce**



References

- **A. Faggionato, F. Martinelli, C. Roberto, C. Toninelli:**
  1. *Aging Through Hierarchical Coalescence in the East Model.* **Comm. in Math. Phys. 309, 459495 (2012)**
  2. *Universality in one dimensional hierarchical coalescence processes.* **Annals of Prob. 40, 1377-1435 (2012)**
  3. *The East model: recent results and new progresses.***Preprint (2012)**
- **P. Chleboun, A. Faggionato, F. Martinelli.** *Time scale separation in the East model.* Forthcoming.