Kinetically constrained particle systems on a lattice

Oriane Blondel

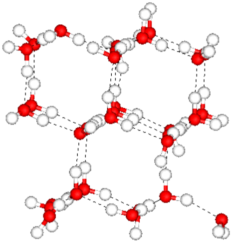
LPMA – Paris 7; ENS Paris

December 3rd, 2013

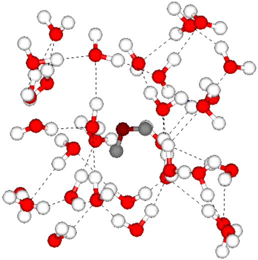
Au commencement était le Verre...


Roland Lagoutte

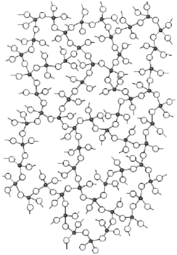
Amorphous solid



Ice



Liquid water



Glass

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- Ingredients
  - Facilitation/geometric constraints
  - No interaction at equilibrium

Toy models for glassy systems

- Ingredients
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  - No interaction at equilibrium
- Can we observe...?
  - Diverging relaxation times
  - Dynamical heterogeneities
  - Breakdown of the Stokes-Einstein relation
  - Etc.

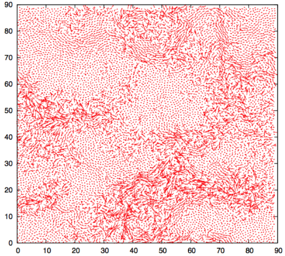

Figure : L. Berthier, Physics 4, 42 (2011)

The models

General description

- Continuous time stochastic processes on $\{0,1\}^{\mathbb{Z}^d}$.
- Transitions = creation/destruction of particles.
- Transition allowed at x only if a local constraint of the type "there are enough zeros around x" is satisfied.
- Density parameter $p \in (0,1)$.

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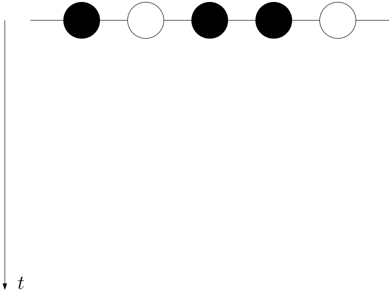
Examples of constraints:

- East model ($d = 1$): the East neighbour should be empty.
- FA-1f* model: there should be at least one empty neighbour.

*Fredrickson-Andersen one-spin facilitated model

Graphical construction (East model, density p)



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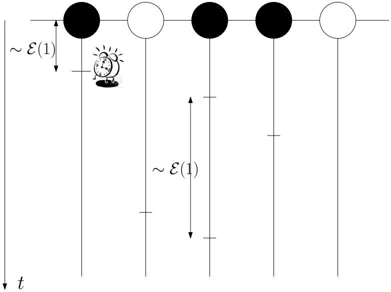

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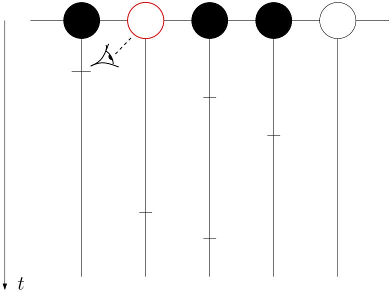

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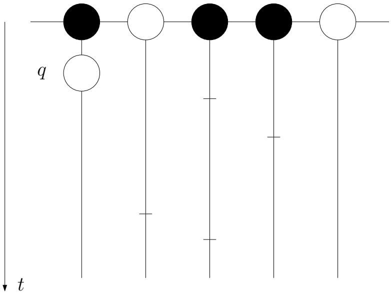

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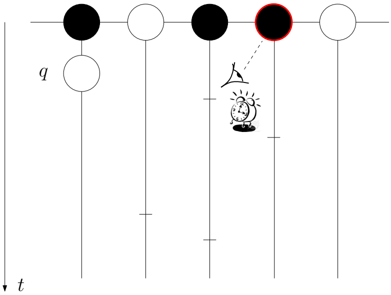

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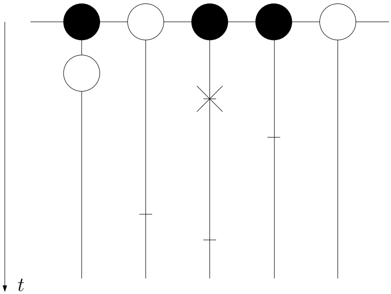

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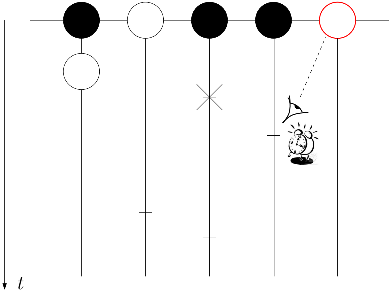

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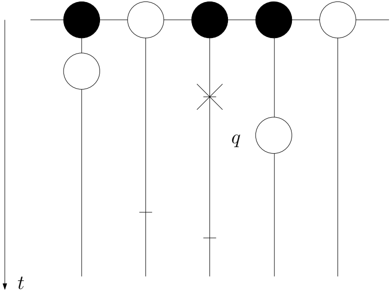

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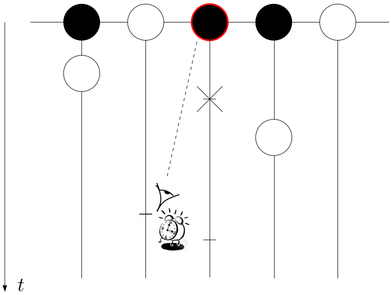

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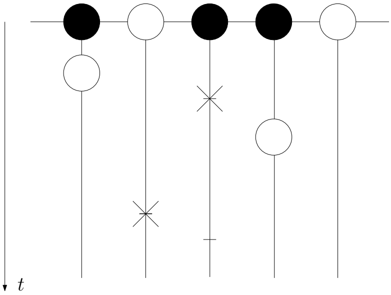

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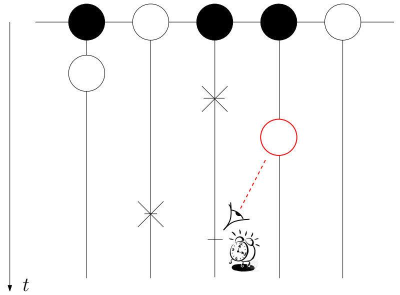

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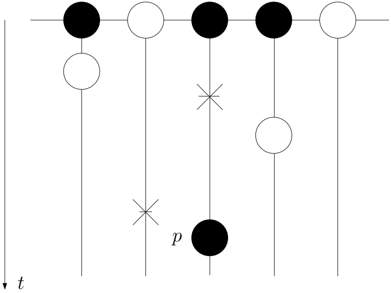

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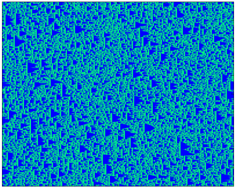
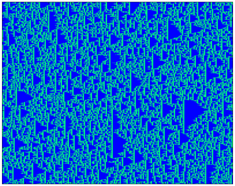
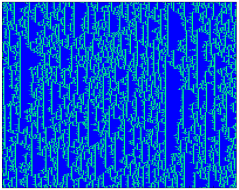
East at different densities



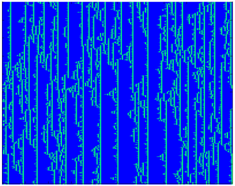
$p = 0.5$



$p = 0.6$



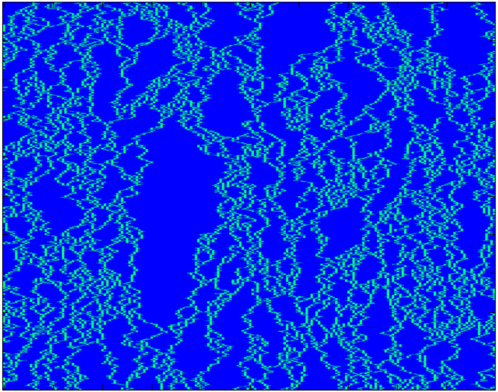
$p = 0.7$



$p = 0.8$

Simulations by Arturo L. Zamorategui.

FA-1f



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Equilibrium

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- Exponential return to equilibrium for East and FA-1f [Aldous-Diaconis '02]

$$Var_\mu(P_t f) \leq Var_\mu(f) e^{-2t/\tau} \quad \text{with} \quad \tau < \infty.$$

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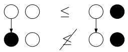
Non-attractive processes: $\eta \leq \sigma \not\Rightarrow \eta(t) \leq \sigma(t)$.



Non equilibrium

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Answer for East: [Cancrini-Martinelli-Schonmann-Toninelli '10]
If η has infinitely many zeros on the right half-line, for all $p \in (0, 1)$

$$|\mathbb{E}_\eta [f(\eta(t))] - \mu(f)| \leq Ce^{-ct} \quad \text{for any local function } f.$$

N.B.: This condition is optimal, since if η has a right-most zero z, for all $t > 0$ $\eta(t)$ remains entirely occupied on the right of z.

Fundamental tool: the distinguished zero.

Out-of-equilibrium relaxation for FA-1f

[B.-Cancrini-Martinelli-Roberto-Toninelli '13, *Markov Proc. Relat. Fields*]

Theorem

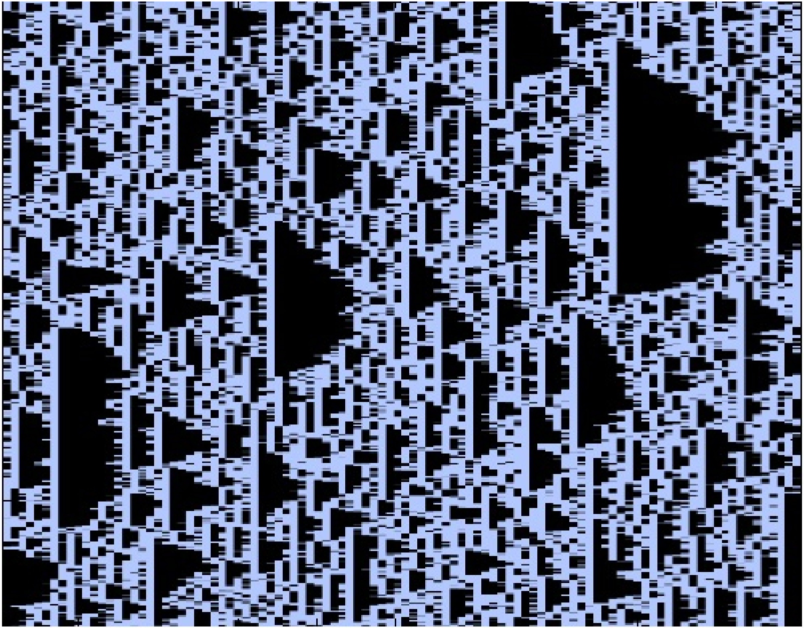
Consider the FA-1f model on $\mathbb{Z}^d$ *with density* p*. Let* μ' *be a probability measure on* Ω*. Assume*

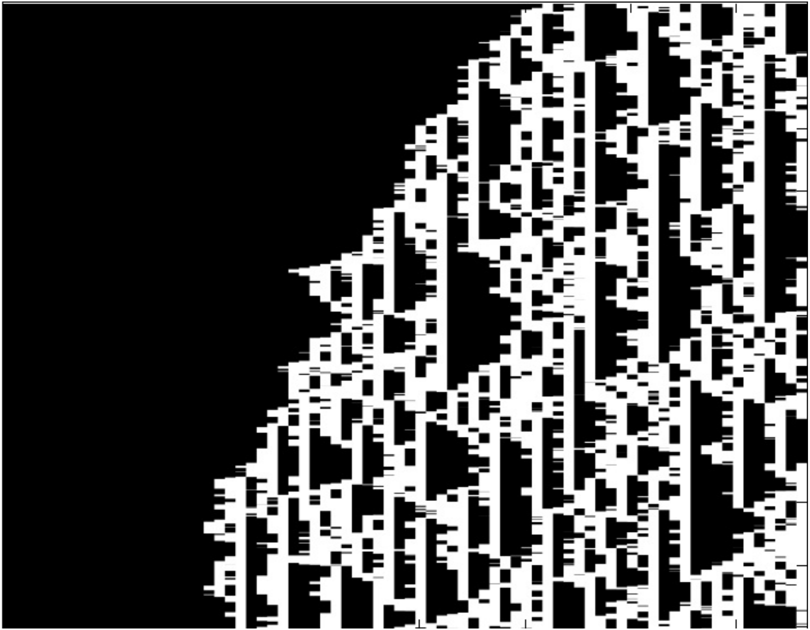
1. $p < 1/2$
2. $\sup_{x\in\mathbb{Z}^d} \mu'\left(\theta^{d(x,\{\text{zeros of }\eta\})}\right) < \infty$ *for some* $\theta > 1$

Then for any local function f *there is a constant* $0 < c < \infty$ *such that*

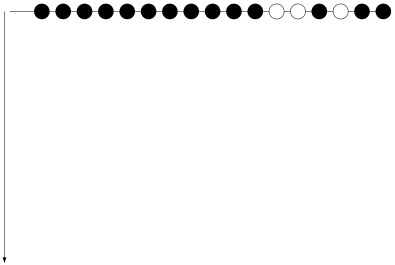
$$|\mathbb{E}_{\mu'}[f(\eta(t))] - \mu(f)| \leq c\|f\|_\infty \begin{cases} e^{-t/c} & \text{if } d = 1 \\ e^{-\left(\frac{t}{c\log t}\right)^{1/d}} & \text{if } d > 1 \end{cases} \tag{1}$$

Bubbles and front





Front progression in the East model



- Start from any configuration with left-most zero at 0.
- Let the East dynamics run for time t.

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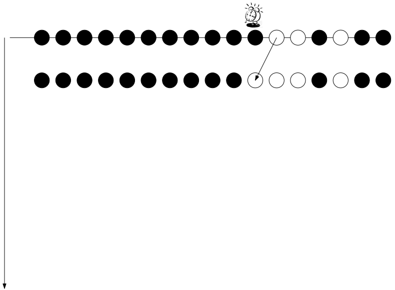

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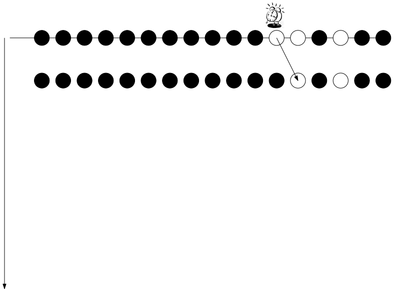

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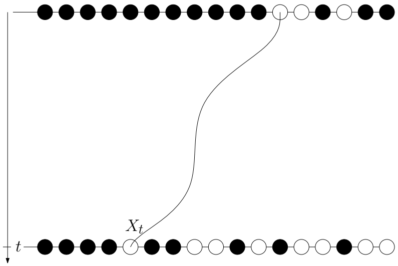

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X_t position of the front (*i.e.* the left-most zero) at time t.
$\theta\eta(t)$ configuration seen from the front at time t.

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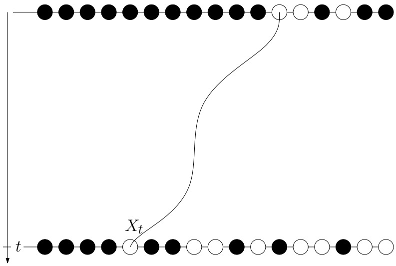

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Questions

- $\frac{X_t}{t} \underset{t\to\infty}{\longrightarrow} v < 0$?
- What does the front see? Invariant measure for $(\theta\eta(t))_{t\geq 0}$? Convergence of $(\theta\eta(t))_{t\geq 0}$?

- μ is not invariant for $(\theta\eta(t))_{t\geq 0}$.

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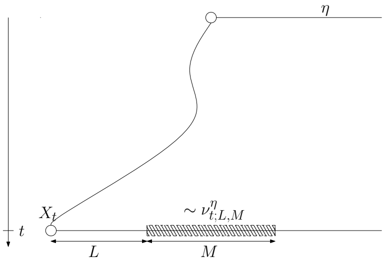
- Dynamics non attractive $\implies$ no subadditive argument.

Central argument

Far from the front, $\theta\eta(t)$ is almost distributed as μ.



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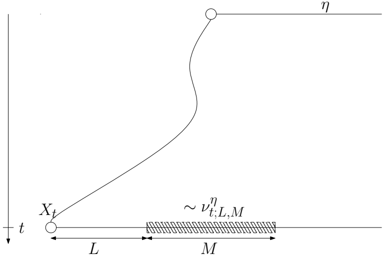
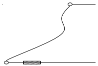
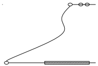


Theorem (B., *SPA* '13)

- *If* $L + M \leq Ct$ 

  $$\|\nu^{\eta}_{t;L,M} - \mu\|_{TV} \leq e^{-\epsilon L}$$

- *If* $L + M > Ct$ *and* η *has "enough zeros"* 

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Perspectives: CLT, large deviations, generalization to non-oriented models.

At low temperature

Questions

- Can we give a simpler description of the dynamics when $q \to 0$?
- Characteristic quantities of the system degenerate when $q \to 0$. How fast? What are the mechanisms involved?

Relaxation time and diffusion

- Relaxation time
  Recall that

$$Var_\mu(P_t f) \leq Var_\mu(f) e^{-2t/\tau} \quad \text{with} \quad \tau < \infty,$$

τ is the relaxation time of the system.

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- Environment: East of FA-1f at equilibrium (initial configuration $\sim \mu$).
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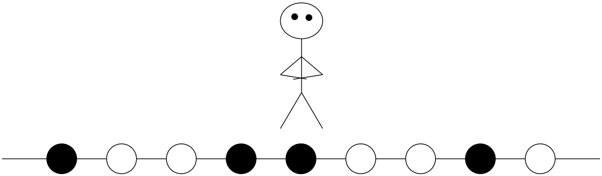

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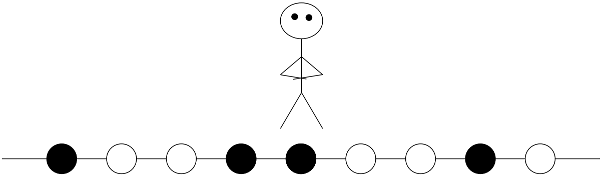

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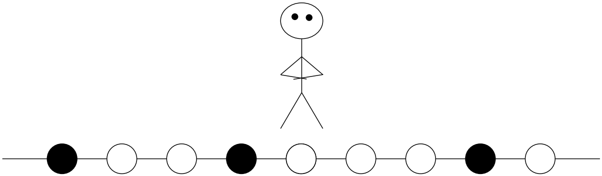

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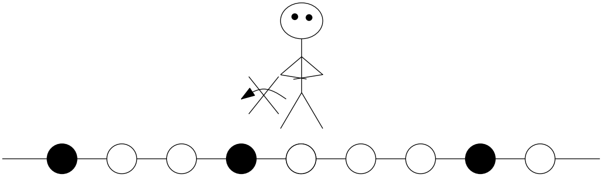

Diffusion coefficient

Setting of [Jung-Garrahan-Chandler '04].

- Environment: East of FA-1f at equilibrium (initial configuration $\sim \mu$).
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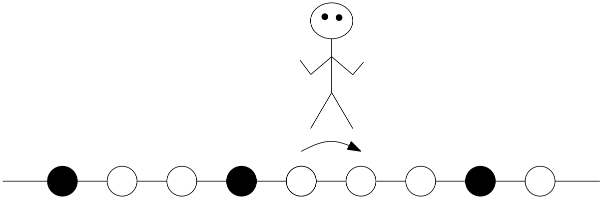

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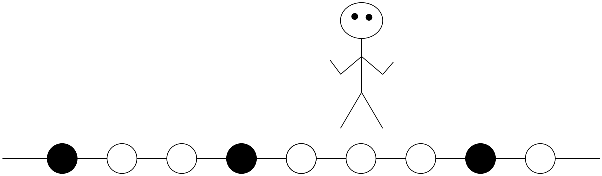

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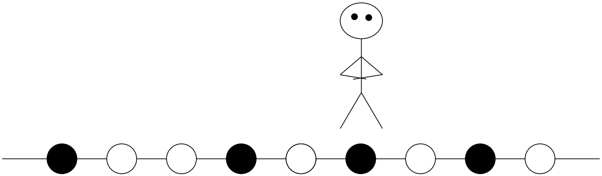

Convergence to Brownian motion

[Kipnis-Varadhan '86, De Masi-Ferrari-Goldstein-Wick '89, Spohn '90]

Proposition

If X_t is the position of the tracer at time t

$$\lim_{\epsilon\to 0} \epsilon X_{\epsilon^{-2}t} = \sqrt{2D} B_t,$$

where B_t is a standard Brownian motion and the diffusion matrix D is given by

$$\begin{aligned} u.Du &= \frac{1}{2}\inf_f \left\{ \sum_{y\in\mathbb{Z}^d} \mu\left(c_y(\eta)((1-q)(1-\eta_y)+q\eta_y)\left[f(\eta^y)-f(\eta)\right]^2\right)\right.\\ &\qquad \left. + \sum_{i=1}^{d}\sum_{\alpha=\pm 1} \mu\left((1-\eta_0)(1-\eta_{\alpha \mathbf{e_i}})\left[\alpha u_i + f(\eta_{\alpha\mathbf{e_i}+\cdot}) - f(\eta)\right]^2\right)\right\}\\ &> 0 \end{aligned}$$

where $u\in\mathbb{R}^d$ and the infimum is taken over local functions f on Ω.

FA-1f at low temperature

- Relaxation time [Cancrini-Martinelli-Roberto-Toninelli '08]

$$
\begin{aligned}
C^{-1}q^{-3} &\leq \tau \leq Cq^{-3} \quad \text{for } d = 1 \\
C^{-1}q^{-2} &\leq \tau \leq Cq^{-2}\log(1/q) \quad \text{for } d = 2 \\
C^{-1}q^{-(1+2/d)} &\leq \tau \leq Cq^{-2} \quad \text{for } d \geq 3
\end{aligned}
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Conjecture: $\tau \sim q^{-2}$ for $d \geq 3$.

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    $\Longrightarrow \xi = 2/3$ if $d=1$, $\xi = 1$ else.

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  - Results of [B. '13]. In all dimensions

$$cq^2 \leq D \leq Cq^2,$$

    and analogous result for other non-cooperative models (with a different, explicit exponent).

East at low temperature

- Relaxation time [AD '02, CMRT '08]

$$c_\delta \exp\left(\frac{\log(1/q)^2}{2\log 2-\delta}\right) \le \tau \le \exp\left(\frac{\log(1/q)^2}{2\log 2+\delta}\right).$$

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  - Prediction of [JGC '04] $D \approx \tau^{-0.73}$.
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  - Results of [B. '13].

$$cq^2\tau^{-1} \leq D \leq Cq^{-\alpha}\tau^{-1} \qquad \Longrightarrow \qquad \frac{\log(D)}{\log(\tau^{-1})} \to 1.$$

Open questions

- Weaker decoupling between D and τ^{-1} in the East model (for instance $D \approx q^{-\alpha}\tau^{-1}$, $\alpha > 0$)?

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- Other KCSM with Stokes-Einstein violation?
- Diffusion when $\tau = +\infty$?

Other perspectives

- Tracer with drift (work in progress, with Luca Avena and Alessandra Faggionato).

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- Tracer with drift (work in progress, with Luca Avena and Alessandra Faggionato).
- Simpler description of FA-1f at low temperature?

Thank you for your attention!

Subadditivity for the contact process.

$\times$: infected, $\square$: healthy.

$\times \to \square$	at rate 1
$\square \to \times$	at rate proportional to the number of infected neighbours.