Kinetically constrained particle systems on a lattice

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LPMA – Paris 7; ENS Paris

December 3rd, 2013
Au commencement était le Verre...
Amorphous solid

Ice

Liquid water

Glass
Toy models for glassy systems

- Ingredients
- Facilitation/geometric constraints
- 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)

O. Blondel

KCSM
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The models
General description

- Continuous time stochastic processes on $\{0, 1\}^Z$.
- 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 $p$)

- Initial configuration $\eta \in \{0, 1\}^\mathbb{Z}$.

- Each site $x$ waits an exponential mean 1 time.
- Then if the constraint is satisfied, $x$ is refreshed to 1 with probability $p$ and 0 w.p. $q = 1 - p$.
- If the constraint is not satisfied, nothing happens.
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Graphical construction (East model, density \( p \))

- Initial configuration \( \eta \in \{0, 1\}^\mathbb{Z} \).
- Each site \( x \) waits an exponential mean 1 time.
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East at different densities

Simulations by Arturo L. Zamorategui.
$p = 0.8$

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Let $\mu = \mathcal{B}(p)^{\otimes \mathbb{Z}^d}$. $\mu$ is reversible for KCSM dynamics and is called the equilibrium measure.

The correlation between $\eta$ and $\eta(t)$ decreases like $e^{-2t/\tau}$ when the initial configuration $\eta$ has law $\mu$. $\tau$ is the relaxation time (inverse of the spectral gap).

Non-attractive processes: $\eta \leq \sigma \neq \Rightarrow \eta(t) \leq \sigma(t)$.
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Exponential return to equilibrium for East and FA-1f [Aldous-Diaconis ’02]

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

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Equilibrium

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\[
\begin{array}{cccc}
\circ & \circ & \circ & \circ \\
\bullet & \circ & \circ & \not\circ
\end{array}
\]
Non equilibrium
What if $\eta \sim \mu', \mu' \neq \mu$? 

N.B.: If $\eta \equiv 1$, at any time $\eta(t) \equiv 1 = \Rightarrow$ no uniform relaxation property.

Better question: given a model, for which density and which initial distribution does the system relax to equilibrium, and at what speed?

Answer for East: [Cancrini-Martinelli-Schonmann-Toninelli '10]

If $\eta$ has infinitely many zeros on the right half-line, for all $p \in (0, 1)$ | $E\eta[f(\eta(t))] - \mu(f) \leq C e^{-ct}$ for any local function $f$.

N.B.: This condition is optimal, since if $\eta$ 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.
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Out-of-equilibrium relaxation for FA-1f


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

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

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

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

(1)
Bubbles and front
Start from any configuration with left-most zero at 0.

Let the East dynamics run for time $t$. 

Questions

- Does $X_t$ converge to $v$ as $t \to \infty$?
- What does the front see? Invariance measure for $(\theta_t)$ $t \geq 0$?
- Does $(\theta_t)$ converge as $t \geq 0$?
Front progression in the East model

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

$X_t$ position of the front (i.e. the left-most zero) at time $t$.

$\theta(t)$ configuration seen from the front at time $t$.

Questions

$X_t \to t \to \infty \Rightarrow v < 0$?

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\( \theta \eta(t) \) configuration seen from the front at time \( t \).
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Questions

- $\frac{X_t}{t} \xrightarrow{t \to \infty} v < 0$?
- What does the front see? Invariant measure for $(\theta \eta(t))_{t \geq 0}$? Convergence of $(\theta \eta(t))_{t \geq 0}$?
\( \mu \) is not invariant for \((\vartheta \eta(t))_{t \geq 0}\).
- $\mu$ is not invariant for $(\theta \eta(t))_{t \geq 0}$.
- Dynamics non attractive $\implies$ no subadditive argument.
Far from the front, $\theta \eta(t)$ is almost distributed as $\mu$. 
Central argument

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

Theorem (B., SPA ’13)

- If $L + M \leq Ct$
  \[ \| \nu_{t;L,M}^\eta - \mu \|_{TV} \leq e^{-\epsilon L} \]

- If $L + M > Ct$ and $\eta$ has “enough zeros”
  \[ \| \nu_{t;L,M}^\eta - \mu \|_{TV} \leq e^{-\epsilon (L \wedge t)} \]
Theorem (B., SPA ’13)

- There exists $v < 0$ such that for every initial $\eta$ as above

\[ \frac{X_t}{t} \xrightarrow{t \to \infty} v \quad \text{in probability}. \]

- The process seen from the front has a unique invariant measure $\nu$ and

\[ \theta \eta(t) \xrightarrow{} \nu \quad \text{in distribution}. \]
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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
  
  $$\text{Var}_\mu (P_t f) \leq \text{Var}_\mu (f) e^{-2t/\tau} \quad \text{with} \quad \tau < \infty,$$

  $\tau$ is the relaxation time of the system.
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- **Diffusion coefficient**
  Add a probe/tracer (*pollen*) to the system (*liquid*) at equilibrium. It diffuses with diffusion coefficient \(D\) depending on the system.
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  In simple liquids,

  \[ D \approx \tau^{-1}. \]
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  In glassy systems,
  \[ D \approx \tau^{-\xi} \quad \text{with} \quad \xi < 1. \]
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For our models?
Diffusion coefficient

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

- Environment: East of FA-1f at equilibrium (initial configuration \( \sim \mu \)).
- Add a tracer at the origin.
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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 $t$

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

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

$$u.Du = \frac{1}{2} \inf_f \left\{ \sum_{y \in \mathbb{Z}^d} \mu \left( c_y(\eta)((1 - q)(1 - \eta y) + q\eta y) \right) \left[ f(\eta^y) - f(\eta) \right]^2 \right\}$$

$$> 0$$

where $u \in \mathbb{R}^d$ and the infimum is taken over local functions $f$ on $\Omega$. 
FA-1f at low temperature

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

\[
C^{-1}q^{-3} \leq \tau \leq Cq^{-3} \quad \text{for } d = 1
\]
\[
C^{-1}q^{-2} \leq \tau \leq Cq^{-2} \log(1/q) \quad \text{for } d = 2
\]
\[
C^{-1}q^{-(1+2/d)} \leq \tau \leq Cq^{-2} \quad \text{for } d \geq 3
\]

Conjecture: \( \tau \sim q^{-2} \) for \( d \geq 3 \).
Relaxation time \cite{Cancrini-Martinelli-Roberto-Toninelli '08}

\begin{align*}
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Diffusion coefficient

- Prediction of \cite{JGC '04} $D \sim q^2$ in all dimensions.

\[ \Longrightarrow \xi = 2/3 \text{ if } d = 1, \xi = 1 \text{ else.} \]
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Diffusion coefficient

- Prediction of [JGC '04] \( D \sim q^2 \) in all dimensions.
  \[ \Rightarrow \xi = 2/3 \text{ if } d = 1, \; \xi = 1 \text{ else.} \]
- 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]

\[ c_\delta \exp \left( \frac{\log(1/q)^2}{2 \log 2 - \delta} \right) \leq \tau \leq \exp \left( \frac{\log(1/q)^2}{2 \log 2 + \delta} \right). \]
East at low temperature

- Relaxation time \([AD '02, CMRT '08]\)

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- Diffusion coefficient
  - Prediction of \([JGC '04]\) \(D \approx \tau^{-0.73}\).
    \(\implies \xi \approx 0.73.\)
Relaxation time \([\text{AD '02, CMRT '08}]\)

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Diffusion coefficient

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  \[\implies \xi \approx 0.73.\]
- Results of \([\text{B. '13}]\).

\[
cq^2 \tau^{-1} \leq D \leq Cq^{-\alpha} \tau^{-1} \quad \implies \quad \frac{\log(D)}{\log(\tau^{-1})} \to 1.
\]
Open questions

- Weaker decoupling between $D$ and $\tau^{-1}$ 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).
Other perspectives

- 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.

•: infected, □: healthy.

• → □ at rate 1
□ → • at rate proportional to the number of infected neighbours.

\[
\begin{align*}
\text{basic coupling} & \quad X^1_s & \quad \eta^1(s) \\
\text{time} & \quad X^1_t & \quad \eta^1(t)
\end{align*}
\]