Stefan problems and kinetically constrained lattice gases

Based on j.w. with O. Blondel, M. Sasada and M. Simon

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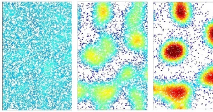
Structure of the talk

1. **Intro: hydrodynamics and KCLG's**
2. **The Facilitated exclusion process**
   - Hydrodynamics for the FEP
   - Equilibrium distributions
   - Estimation of the transience time
3. **Higher dimension and boundary interactions**
   - CLG_2 and FEP_2
   - Diffusion coefficient and reservoirs
4. **Comments and (some) open problems**

Statistical physics and hydrodynamic limits

Linking micro/macro levels of description for a variety of physical systems to prove phase transition phenomena for out of equilibrium systems. Some examples :

- **Active matter** models : spontaneous condensation (MIPS) and onset of collective motion (travelling waves).

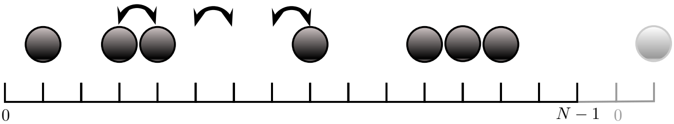


- **Non-equilibrium** models, e.g. boundary-driven systems.

- **Kinetically constrained lattice gases** to model the liquid-solid phase transition.

An elementary example : Symmetric Simple Exclusion Process (SSEP)

- Bulk $\Lambda_N = \{0, \ldots, N-1\}$ with periodic boundary conditions.
- Configuration $\eta \in \Omega_N := \{0,1\}^{\Lambda_N}$, with $\eta_x = 1$ for an occupied site, $\eta_x = 0$ for an empty site.
- *Stirring dynamics*: two neighboring sites are exchanged at rate 1.



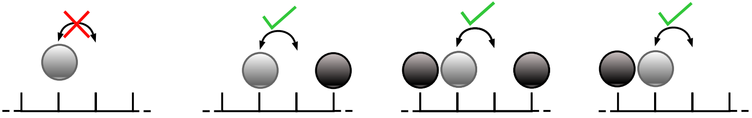
Assuming that the initial configuration $\eta(0)$ is "close" to a macroscopic profile $\rho_0 : [0,1) \to [0,1]$, the macroscopic evolution of the system is ruled by the heat equation

$$\begin{cases} \partial_t \rho = \partial_{uu}\rho \\ \rho(0,\cdot) = \rho_0 \end{cases},$$

where ρ is the density field, "$\rho(t,u) = \mathbb{E}(\eta_{uN}(tN^2))$".

Kinetically Constrained Lattice Gases

Question: What happens if a kinetic constraint is added to the dynamics ?
Example: *[Gonçalves, Landim, Toninelli '08]*:



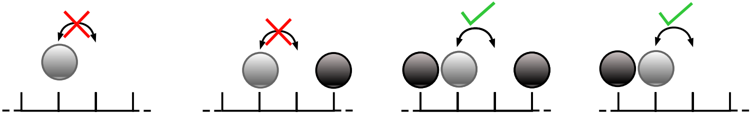
With the right jump rates, the hydrodynamic behavior for this macroscopic system is ruled by the *porous medium equation*

$$\begin{cases} \partial_t \rho = \partial_{uu}\, \rho^2 \\ \rho(0,\cdot) = \rho_0 \end{cases} .$$

- Bernoulli product measures are reversible for this process.
- *Mobile cluster*: two consecutive particles can move around the system and locally mix the system. $\mapsto$ local ergodicity.

Facilitated Exclusion Process (FEP)

Stronger kinetic constraint than in *[Gonçalves, Landim, Toninelli '08]*: A particle can jump to a neighbor site iff its other neighbor is occupied.



Markov generator:

$$\mathcal{L}_N f(\eta) = \sum_{x \in \Lambda_N} c_{x,x+1}(\eta)\{f(\eta^{x,x+1}) - f(\eta)\},$$

with

$$c_{x,x+1}(\eta) = \eta_{x-1}\eta_x(1-\eta_{x+1}) + \eta_{x+2}\eta_{x+1}(1-\eta_x),$$

and $\eta^{x,x+1}$ is the configuration where sites x and $x+1$ have been exchanged.

- Bernoulli product measures are not stationary.
- No longer a *mobile cluster* to mix the configuration.

Hydrodynamic limit for the FEP

We start the process from a product measure μ_N "fitting" a macroscopic profile $\rho_0 : [0,1] \to [0,1]$, i.e. $\mu_N(\eta_x = 1) = \rho_0(x/N)$.

Theorem (Blondel, E', Simon, Sasada 2018 & BES 2021)

Consider the process $\eta(t)$ started from the measure μ_N, and driven by $N^2\mathcal{L}_N$. Given an initial profile ρ_0, we have for any test function H

$$\frac{1}{N}\sum_{x\in\Lambda_N} H(x/N)\eta_x(t) \xrightarrow[N\to\infty]{\mathbb{P}} \int_{[0,1]} H(u)\rho(t,u)du$$

where ρ is solution to the Stefan problem $\rho(0,u) = \rho_0(u)$ and

$\boxed{\rho_0 > 1/2}$

$$\partial_t \rho = \partial_{uu}\left\{\frac{2\rho - 1}{\rho}\right\}$$

$\boxed{\rho_0 \in [0,1]}$

$$\partial_t \rho = \partial_{uu}\left\{\frac{2\rho - 1}{\rho}\mathbf{1}_{\{\rho\geq 1/2\}}\right\}.$$

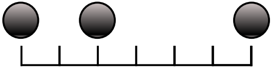
Types of configurations

Define $\Omega_N^k = \{\eta \in \Omega_N,\ \sum \eta_x = k\}$, there are four types of configurations:

- *If* $k \leq N/2,\ \Omega_N^k = F_N^k \cup TB_N^k$:

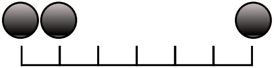
Frozen configurations

$$F_N^k = \{\eta \in \Omega_N^k \ \mid \ \eta_x \eta_{x+1} \equiv 0\}$$



Transient Bad configurations

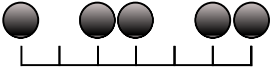
$$TB_N^k = \{\eta \in \Omega_N^k \ \mid \ \eta_x \eta_{x+1} \not\equiv 0\}.$$



- *If* $k \geq N/2,\ \Omega_N^k = E_N^k \cup TG_N^k$:

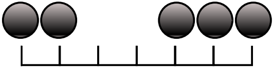
Ergodic configurations

$$E_N^k = \{\eta \in \Omega_N^k \mid (1-\eta_x)(1-\eta_{x+1}) \equiv 0\}$$



Transient Good configurations

$$TG_N^k = \{\eta \in \Omega_N^k \mid (1-\eta_x)(1-\eta_{x+1}) \not\equiv 0\}$$



Equilibrium distributions

For $k \geq N/2$, the uniform distribution π_N^k on E_N^k satisfies *detailed balance*, and is therefore a reversible measure for the process on E_N^k, so that one only needs to compute $|E_N^k|$.

To do so, two possibilities for the first site of the configuration:

- If occupied, we have $N-k$ empty sites, to be placed in k interstices between particles.
- If empty, it is surrounded by particles, and we have $N-k-1$ empty sites, to be placed in $k-1$ interstices between particles.

$$|E_N^k| = \binom{k}{N-k} + \binom{k-1}{N-k-1}$$

Grand canonical measures

With similar combinatorial arguments, given a configuration σ on a box $\{1, \dots, \ell\}$, one can compute

$$\pi_N^k(\eta_{|\{1,\dots,\ell\}} = \sigma) = \frac{\left|\left\{\eta \in E_N^k, \eta_{|\{1,\dots,\ell\}} = \sigma\right\}\right|}{|E_N^k|}.$$

As $N \to \infty$ and $k/N \to \rho > 1/2$,

$$\pi_N^k(\eta_{|\{1,\dots,\ell\}} = \sigma) \underset{N\to\infty}{\longrightarrow} \pi_\rho(\eta_{|\{1,\dots,\ell\}} = \sigma)$$

defines the grand canonical measure π_ρ on the set of infinite ergodic configurations.

- π_ρ is supported on the infinite ergodic component.
- π_ρ is a Bernoulli product measure conditioned to having isolated empty sites (ergodic component)
- π_ρ exhibits **long-range correlations** as $\rho \searrow 1/2$.

Entropy tools and equilibrium distributions

The most classical techniques for hydrodynamic limits are based on **entropy bounds** between the measure μ_t^N of the process at time t and its reference measures π_α, namely

- Guo, Papanicolaou and Varadhan's **entropy method**,

$$H(\mu_t^N \mid \pi_\alpha) \leq CN,$$

- Yau's **relative entropy method**

$$H(\mu_t^N \mid \pi_{\rho_t}) = o(N).$$

Supercritical case, in the transient regime, μ_t^N is not supported on ergodic configurations, whereas the grand canonical measures π_ρ are $\Rightarrow$ entropy estimate fails. In particular, we need to prove that the ergodic component is reached quicker than the diffusive timescale $\tau = O(N^2)$.

General case, no hope of using the entropy method : no reference measures because the two phase's stationary states have **disjoint supports**.

Estimation of the transience time

Theorem (Thermalization of the supercritical phase, BESS18)

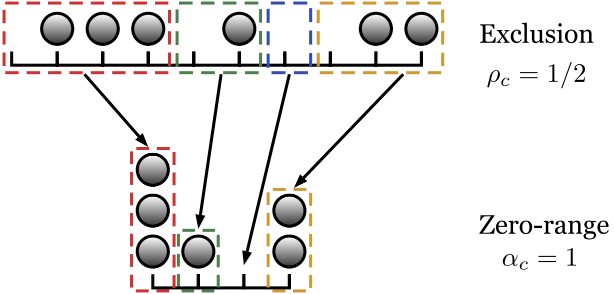
Assume that $\rho_0 > 1/2$. There exists α such that, letting $t_N = (\log N)^\alpha / N^2$ and k_0 the initial number of particles in the configuration,

$$\lim_{N\to\infty} \mathbb{P}(\eta(t_N) \notin E_N^{k_0}) = 0.$$

Theorem (Thermalization in a general case, BES21)

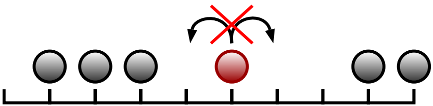
- *The ergodic and frozen phases thermalize w.h.p in a time of order* $t_N = (\log N)^\alpha / N^2$.
- *A critical interface a, assuming $\partial_u \rho_0(a) \neq 0$ thermalizes w.h.p in a time of order* $t_N = N^{-\varepsilon}$.
- *Otherwise, (i.e. if $\partial_u \rho_0(a) = 0$), the "thermalization time" t_N is $O(1)$.*

Transience time : mapping with a ZR process

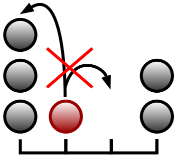


- This zero-range process is **attractive**.
- To understand the **supercritical** transience time, one need to estimate the time the zero-range takes to **fill all empty sites** in the supercritical region.
- To understand the **subcritical** transience time, one needs to estimate the time the zero-range takes for all particles to **fall in an empty site**.

Transience time : mapping with a ZR process



Exclusion
$\rho_c = 1/2$



Zero-range
$\alpha_c = 1$

- This zero-range process is **attractive**.
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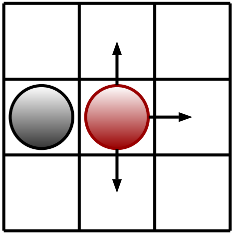
$\boxed{\rho_0 \in [0,1]}$

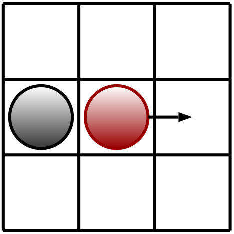
$$\partial_t \rho = \partial_{uu}\left\{\frac{2\rho - 1}{\rho}\mathbf{1}_{\{\rho\geq 1/2\}}\right\}.$$

- Supercritical case $\rho_0 > 1/2$: thermalization+ properties (*decorrelation, equivalence of ensembles*) of $\pi_\rho, \pi_N^k \implies$ Hydrodynamic Limit (Entropy Method, Guo, Papanicolaou, Varadhan, '88)
- General case $\rho_0 \in [0,1]$: proved adapting a result by Funaki '99. Requires some De Finetti type result on the decomposition of translation invariant stationary measures for the process.

Analogous models in dimension d=2



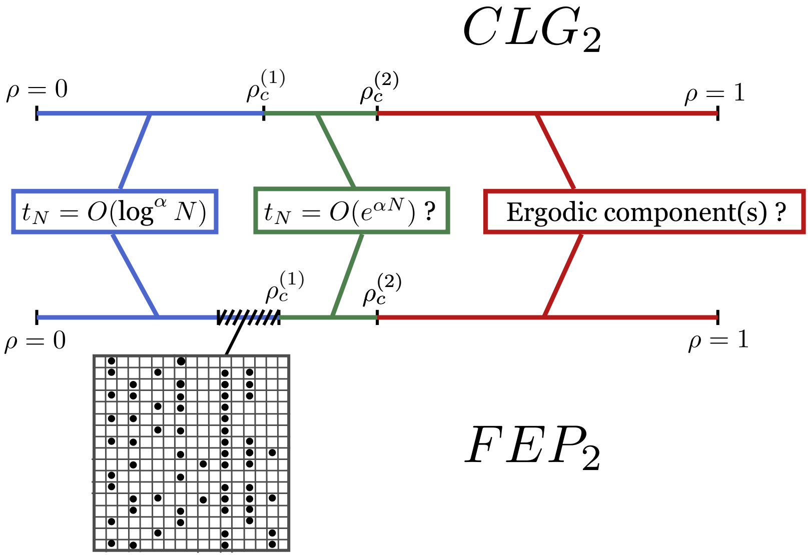
CLG_2



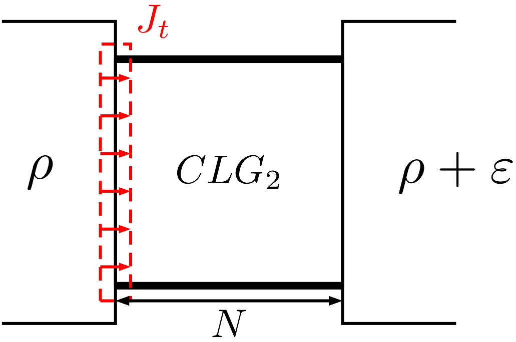
FEP_2

- In two dimensions, several critical density threshold : threshold for **ergodicity**, threshold for **subdiffusive transience**.
- All tools developed for dimension 1 fail, zero-range mapping no longer available : hydrodynamic behavior out of reach.
- for FEP_2, another critical density with onset of quasi-1-dimensional behavior for $\rho \leq 1/4$

CRITICAL DENSITIES FOR CLG_2 AND FEP_2



Diffusion coefficient and reservoir interaction



For the diffusion coefficient $D(\rho)$ of the $2d$ system, with “hydrodynamics”

$$\partial_t \rho = \nabla \cdot D(\rho) \nabla \rho,$$

the following gives a concrete computation scheme;

- System in contact with two reservoirs, left density ρ, right density $\rho + \varepsilon$
- Stationary regime: left boundary total current $J_t \simeq -NtD(\rho)\nabla_{0,1}\rho$.

$$\implies D(\rho) = -\lim_{t\to\infty} \lim_{\varepsilon\to 0} \frac{J_t}{t\varepsilon}.$$

Reservoir interaction and hydrodynamics

- When a particle system is affected by a non-conservative reservoir dynamics with equilibrium density α, The hydrodynamic will typically exhibit **Dirichlet boundary conditions** with the same value α as the reservoir.

- For exclusion dynamics, a typical reservoir dynamics consists in filling an empty site at rate α and emptying an occupied site at rate $1-\alpha$.

- In the case of kinetically constrained models, the interplay between boundary dynamics and bulk dynamics is less straightforward because of the **frozen phase**.

- In the frozen phase, there is no diffusion until the system locally reaches the critical density. In particular, a subcritical reservoir dynamics $\alpha < \rho_c$ will, microscopically enforce a **supercritical effective density** $\alpha_{\text{eff}} > \rho_c$.

Diffusion coefficient and reservoir interaction

- It seems like the diffusion coefficient is continuous on $\rho \in [0, 1]$.
- The definition of the diffusion coefficient itself is problematic, since there is no diffusion under density $\rho_c \simeq 1/3$
- Even subcritical reservoirs enforce an **effective supercritical density**, and this density is larger than ρ_c
- Delicate interpretation of this quantity in the subcritical regime.

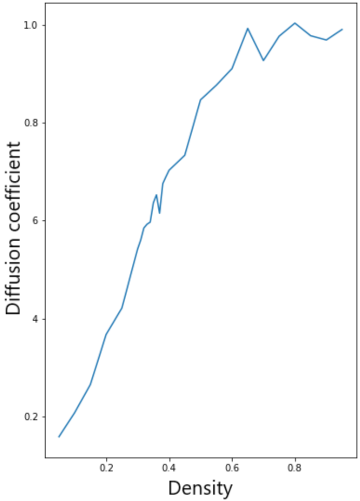


Figure: Simulation by A. Roget

Comments and open problems

- ▷ Hydrodynamic limit result in **one dimension with subcritical reservoirs** ?
- ▷ Starting from an empty configuration with subcritical reservoir, **front progression** on a timescale $t = O(N^3)$?
- ▷ Explicit expression and characterization of **critical densities** 2 dimensions ? Can we uncover the **structure of the ergodic configurations** ?
- ▷ Can we tackle **other kinetic constraints**, in dimension 1 ? Is there an analogous separation in ergodic/frozen phases ?