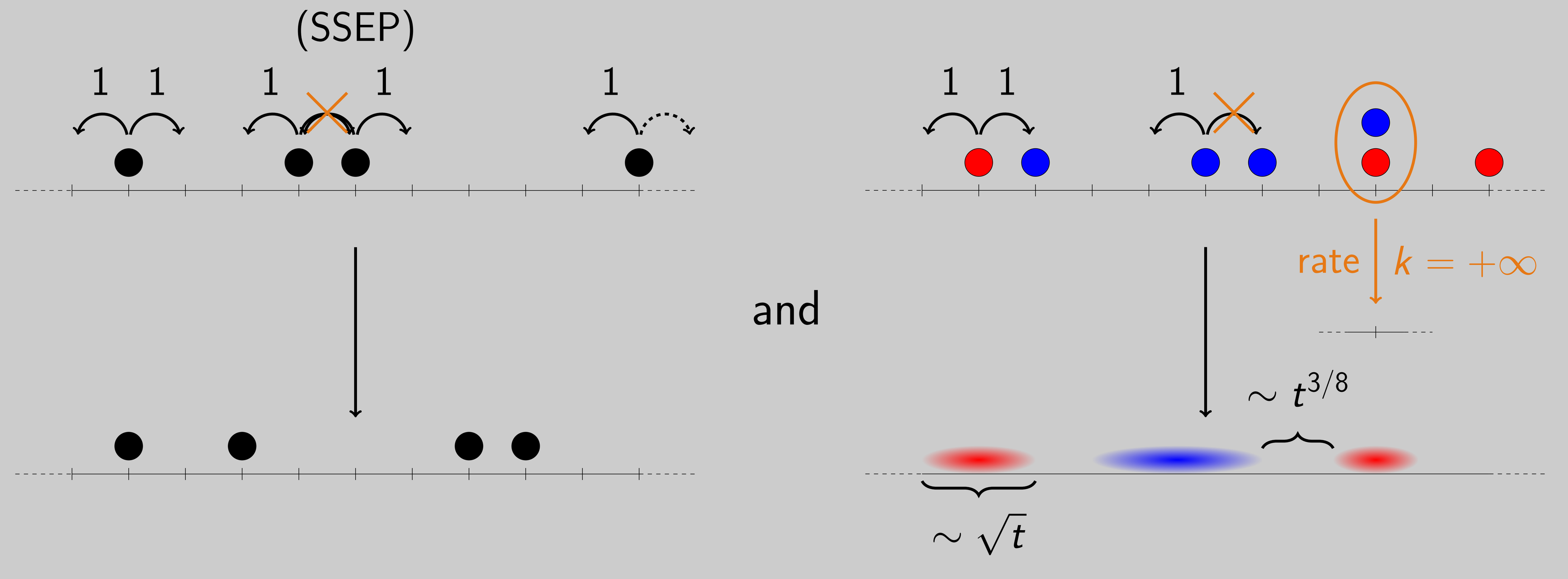
From exclusion to pair annihilation

Tanguy Laffargue[1], Peter Sollich[2], Julien Tailleur[1], Frédéric van Wijland[1]

1. Laboratoire Matière et Systèmes Complexes, Université Paris Diderot
2. Department of Mathematics, King's College London

Is there anything in common between

Symmetric Simple Exclusion Process (SSEP) and $A + B \to \emptyset$



Total density: $\rho(t) = \rho_0$ at all time.

Total density: $\rho(t) \sim t^{-1/4}$.

The answer is yes and here is why.

SSEP and fluctuating hydrodynamics

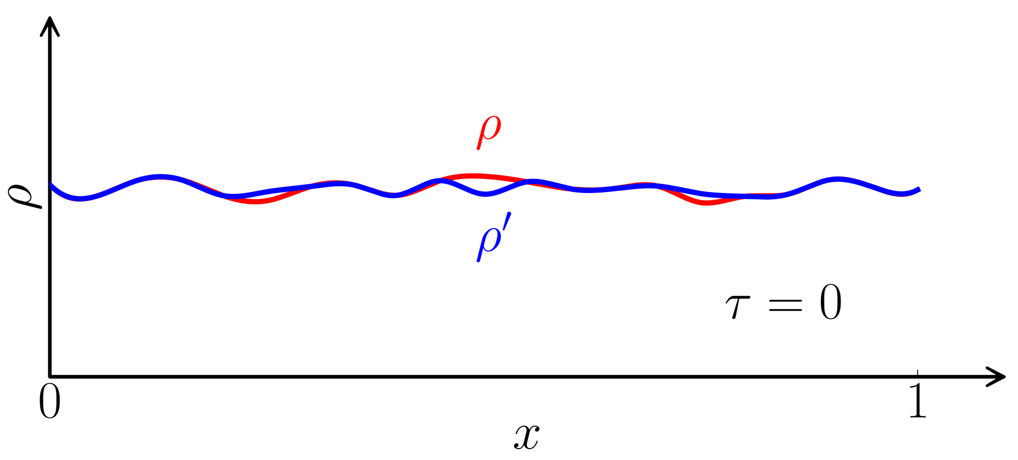
Size L, total time t, periodic boundary conditions (PBC)

$$\begin{cases} n_i(t') = 0 \text{ or } 1 \\ i = 1, 2, \dots, L \\ 0 \leqslant t' \leqslant t \end{cases} \xrightarrow{\text{large } L} \begin{cases} \text{“}\rho(x,\tau) = n_i(t')\text{”} \\ x = i/L \\ \tau = t'/L^2 \text{ and } T = t/L^2 \end{cases}$$

Fluctuating hydrodynamics:

$$\partial_\tau \rho(x,\tau) = -\partial_x j(x,\tau), \quad j(x,\tau) = \underbrace{-\partial_x \rho}_{\text{Fick's law}} + \underbrace{\sqrt{\frac{2\rho(1-\rho)}{L}}\,\overbrace{\xi(x,\tau)}^{\text{Gaussian white noise}}}_{\text{fluctuations}}$$

Chaos and fluctuating Lyapunov exponent



How does the difference between initially close-by configurations evolve?

$$u = \rho - \rho'$$

$$|u| \underset{\text{large } \tau}{\sim} e^{\tau\lambda(\tau)}$$

λ is the largest Lyapunov exponent (associated to the density). It characterizes the stability/chaoticity of the system:

- $\lambda > 0 \Rightarrow |u|$ grows: the system is chaotic.
- $\lambda < 0 \Rightarrow |u| \to 0$: the system is stable.

What is the pdf of $\lambda(T)$? Compute $Z(\alpha, \tau)$, the moment-generating function.

Methods: field theory and Saddle-Point approximation

Field theory using the MSRJdD formalism:

$$Z(\alpha, T) = \langle e^{-\alpha L T \lambda(T)} \rangle = \int \mathcal{D}[\rho, \bar\rho, v, \bar v, \mu, \kappa, \eta]\ e^{-LS[\rho,\bar\rho,v,\bar v,\mu,\kappa,\eta]}$$

with:

$$S = \int_0^T \mathrm{d}\tau \int_0^1 \mathrm{d}x \left[\bar v\, \partial_\tau v + D\, \partial_x v\, \partial_x \bar v - D \left(\alpha + \int_0^1 \mathrm{d}y\ v \bar v \right) (\partial_x v)^2 + \bar\rho\, \partial_\tau \rho + D\, \partial_x \rho\, \partial_x \bar\rho \right.$$
$$\left. - \frac{\sigma'^2}{8\sigma} \left(v\, \partial_x \bar v - \left(\alpha + \int_0^1 \mathrm{d}y\ v \bar v \right) v\, \partial_x v + \frac{2\sigma}{\sigma'} \partial_x \bar\rho \right)^2 + \mu\,(\rho - \rho_0) + \kappa\, v + \eta\,(v^2 - 1) \right]$$

Large deviation principle:

$$Z(\alpha, T) \underset{\substack{T\to\infty \\ L\to\infty}}{\sim} e^{LT\psi(\alpha)}$$

We want to determine the dynamical free energy $\psi(\alpha)$.

Variable	Equilibrium statistical physics	Dynamical system
“Temperature”	β	α
Partition function	$Z(\beta) = \langle e^{-\beta E} \rangle$	$Z(\alpha) = \langle e^{-\alpha L T \lambda} \rangle$
Free energy	$f(\beta) = \frac{1}{\beta L} \ln(Z)$	$\psi(\alpha) = \frac{1}{TL} \ln(Z)$

α is the temperature for the chaoticity:

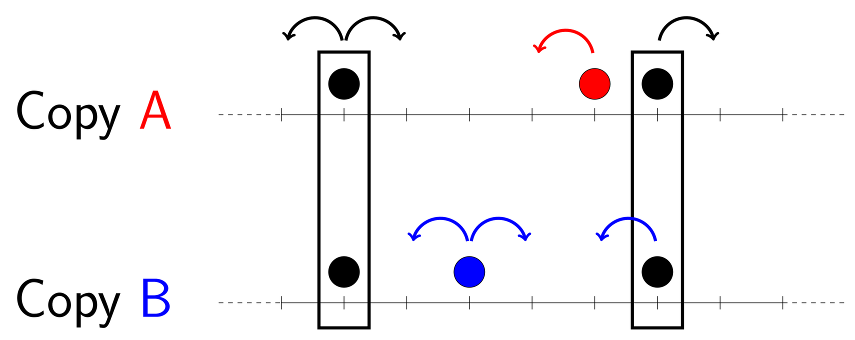
- $\alpha > 0$: favoring stable trajectories
- $\alpha < 0$: favoring chaotic trajectories

Saddle-Point approximation, valid for $\alpha < 0$:

$$\psi(\alpha) = 4\pi^2\alpha \left[1 + \frac{1}{8} \frac{(1-2\rho_0)^2}{\rho_0(1-\rho_0)} \alpha + \frac{3}{128} \left(\frac{(1-2\rho_0)^2}{\rho_0(1-\rho_0)} \alpha \right)^2 + \mathcal{O}(\alpha^3) \right]$$

Discrete version

Two copies of the SSEP with the same dynamics. What does “same noise” mean? Noise caused by the environment (for instance by the solvent) $\Rightarrow$ noise depends on site.

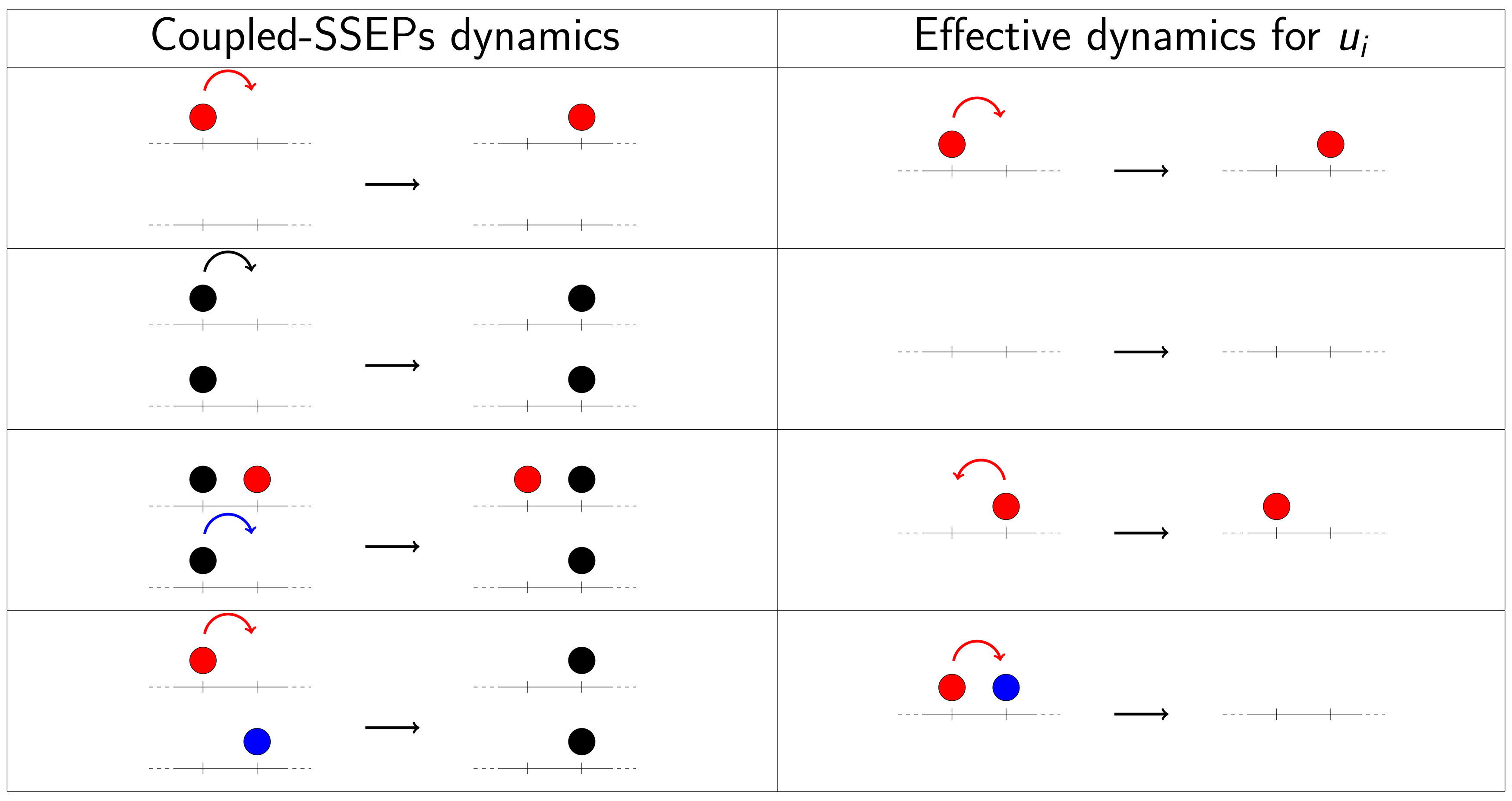


Possible jumps (all with rate 1):

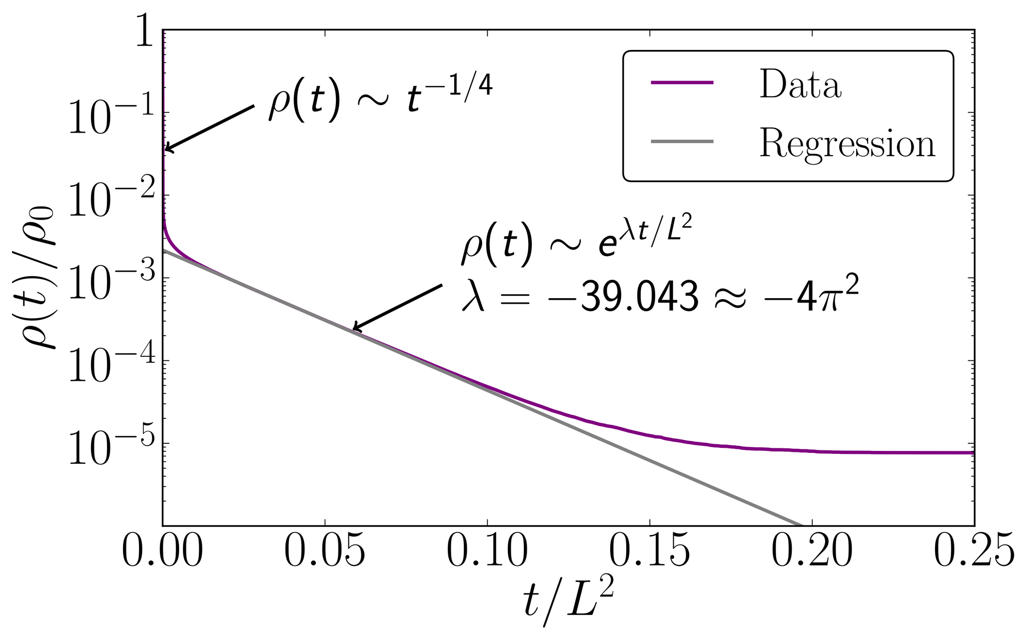
- particle jumping in system A (red)
- particle jumping in system B (blue)
- particle jumping in both systems at the same time (black)

Mapping to $A + B \to \emptyset$

In the two coupled SSEPs, we are interested in the difference between the two systems $u_i(t') = n_i^A(t') - n_i^B(t')$. Sites occupied in both systems (•) are not contributing, and we focus on the distribution of sites occupied only in A (•) or only in B (•). We can then define an effective dynamics by removing the non-contributing particles.



We can see that the effective dynamics, describing the u_i dynamics with the connection (• $\leftrightarrow u_i = +1$) and (• $\leftrightarrow u_i = -1$), is equivalent to $A + B \to \emptyset$ with exclusion and an infinite reaction rate.



Numerical simulation of the $A + B \to \emptyset$ reaction-diffusion process using the Renormalized Reaction-Cell method (developed by D. ben-Avraham). The system has 2^{20} sites, the initial density of each kind of particle is 0.125 and this graph is an average over 1000 runs.

Conclusion

- Technique to access chaotic properties in many body interacting systems.
- New results on $A + B \to \emptyset$ in finite size, bearing on a distribution function rather than on an average.
- A definition, reminiscent of damage spreading, for a Lyapunov exponent in a system with discrete degrees of freedom.

tanguy.laffargue@univ-paris-diderot.fr