Diffusion in a simplified random Lorentz gas

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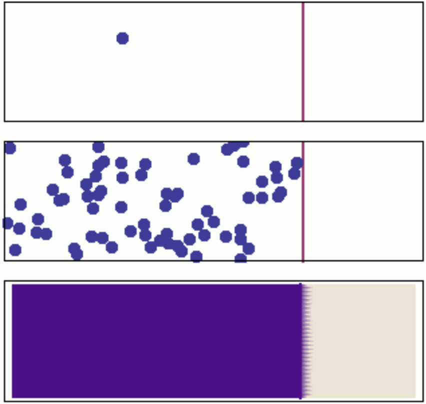
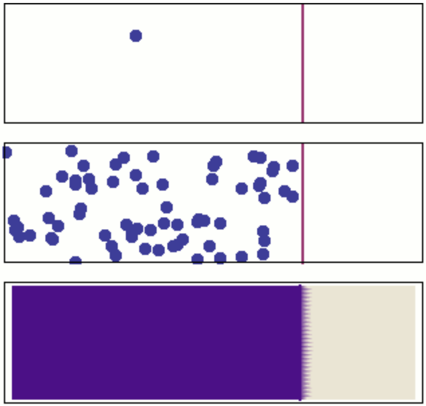
Mathematical Statistical Physics in Kyoto 2013.

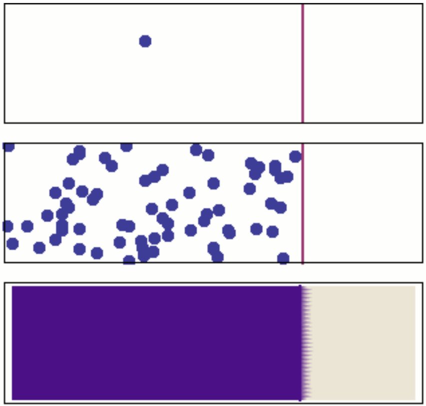
Goal: Introduce a new model designed to derive macroscopic diffusion from a deterministic (but with random parameters) microscopic dynamics in a “‘typical” sense.

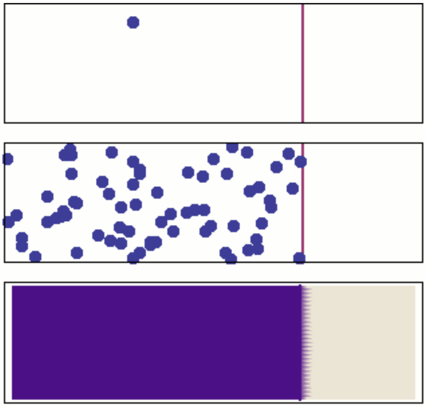
RL *Macroscopic diffusion from a Hamilton-like dynamics*
Journal of Statistical Physics, Volume 151 (5),861-869 (2013)

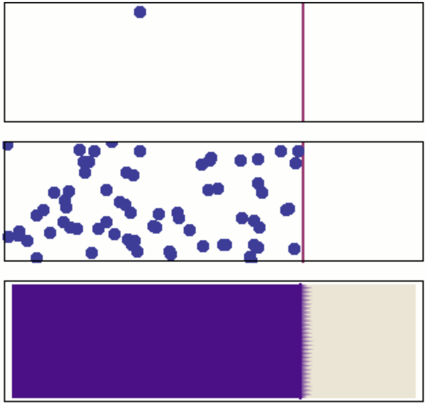
Diffusion of particles : Fick's law

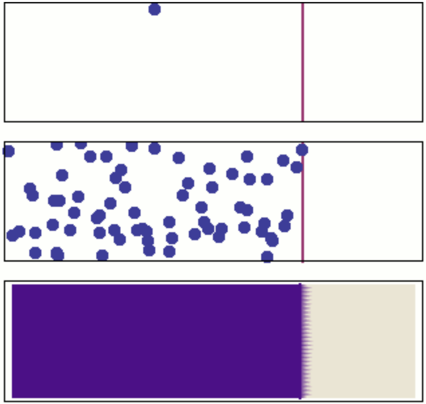


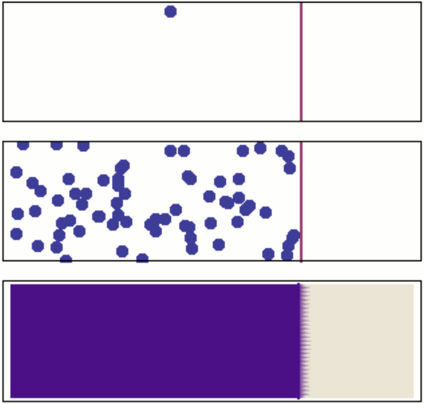


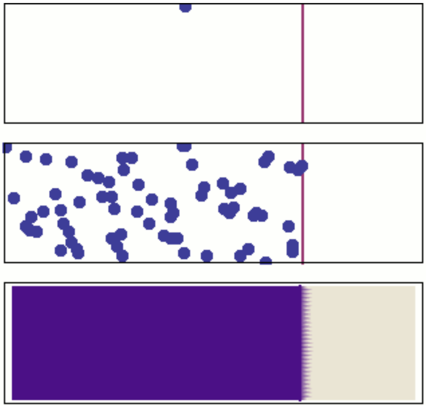


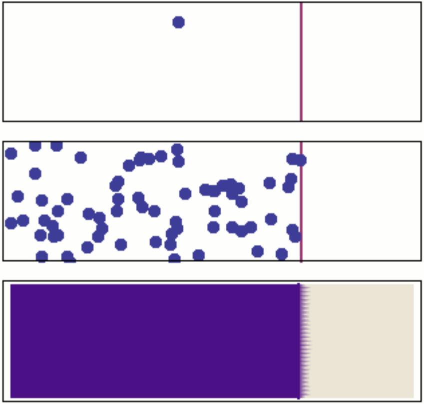


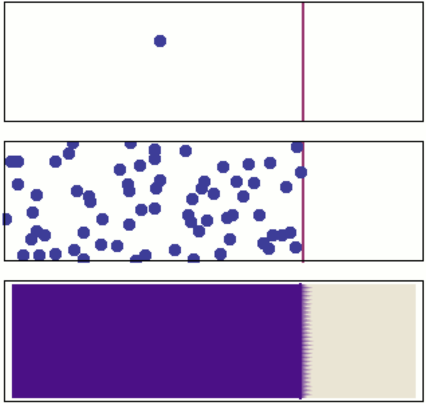


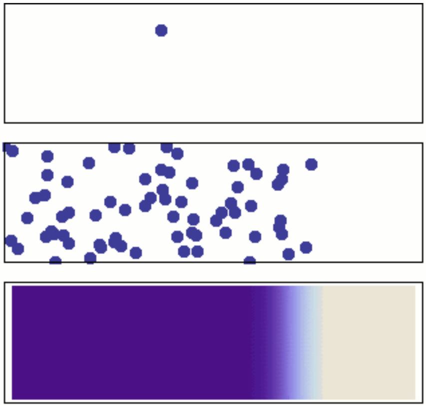


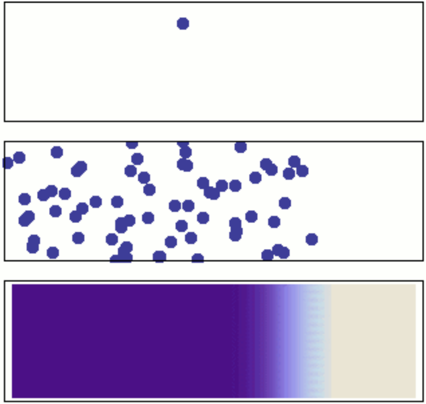


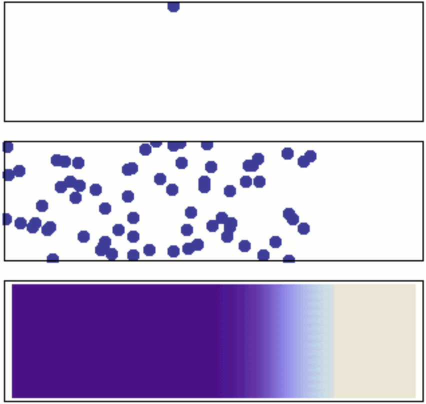


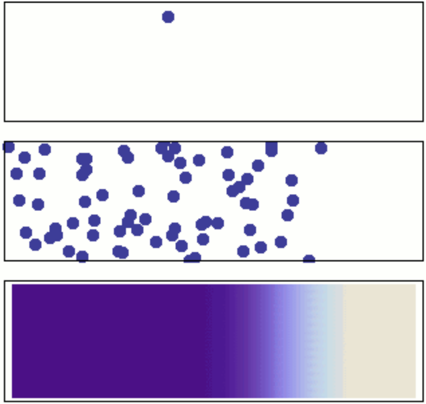


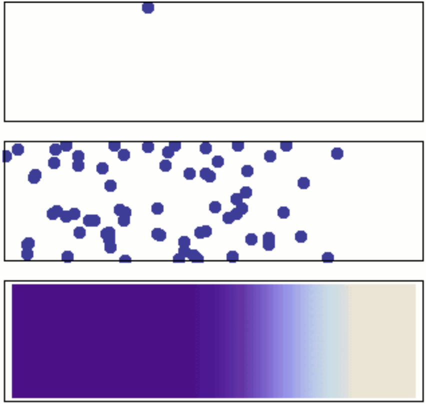


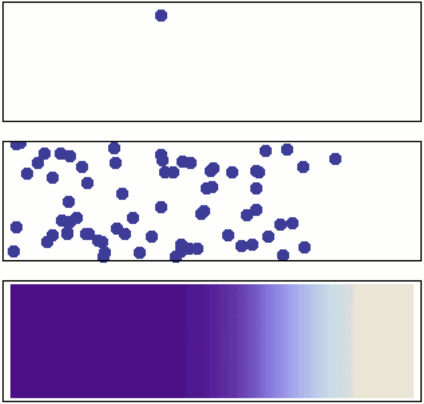


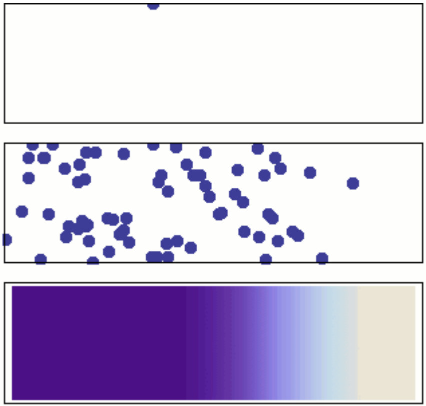


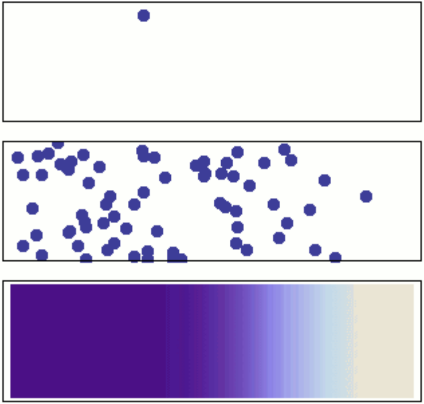


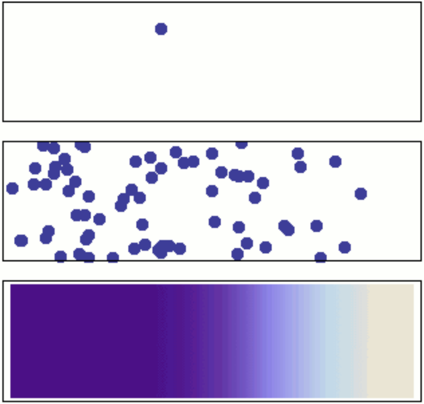


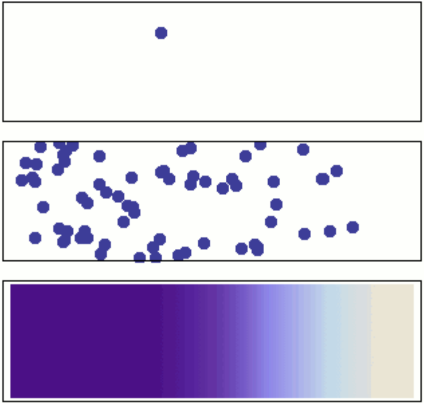


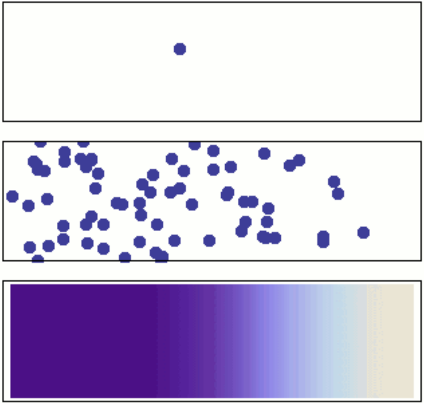


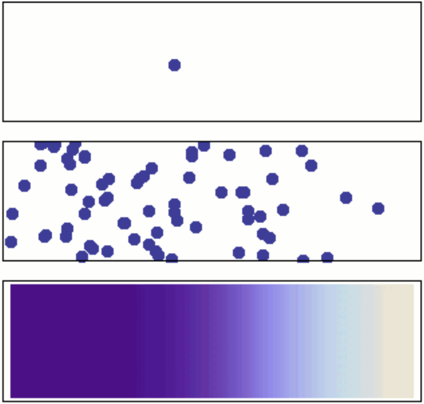


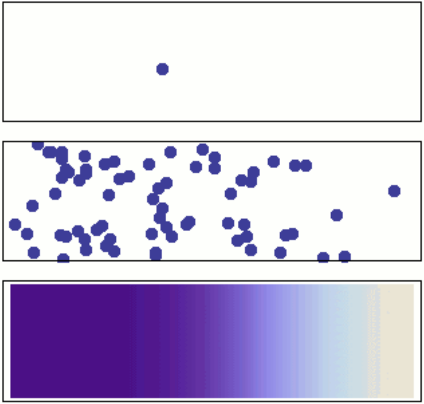


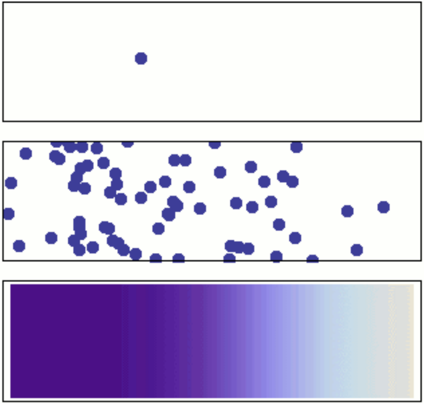


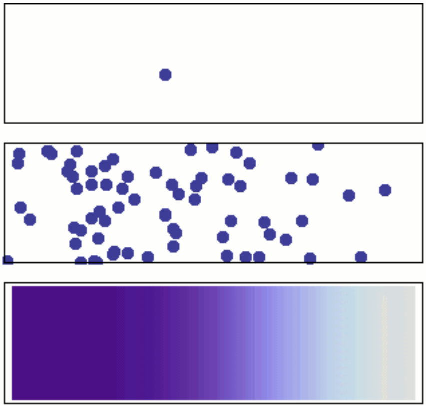


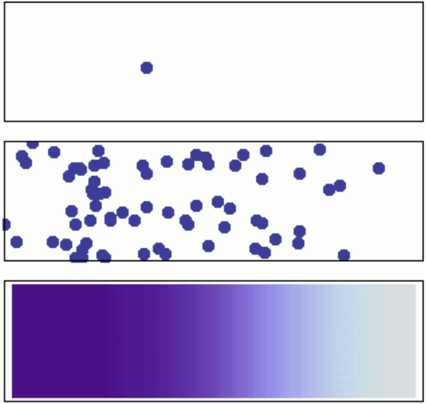


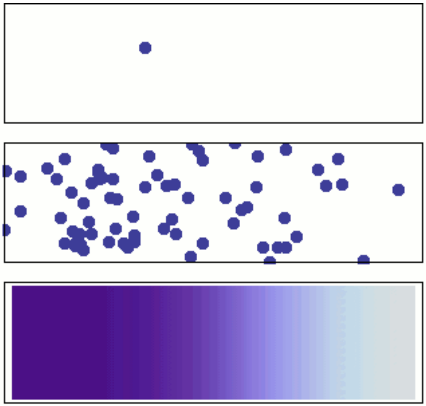


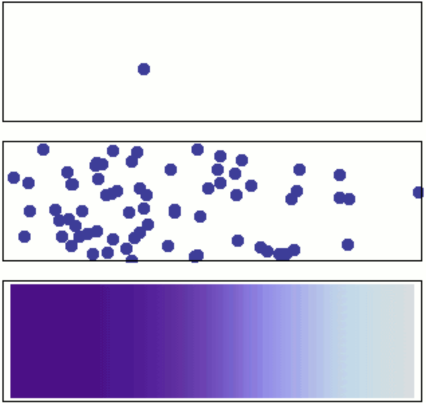


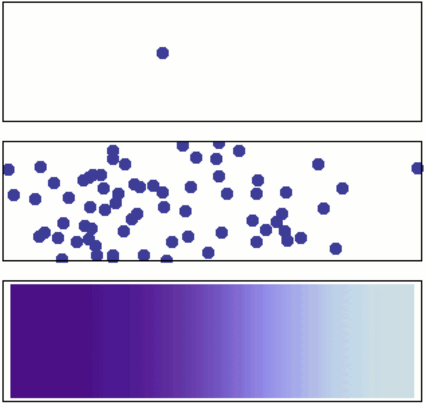


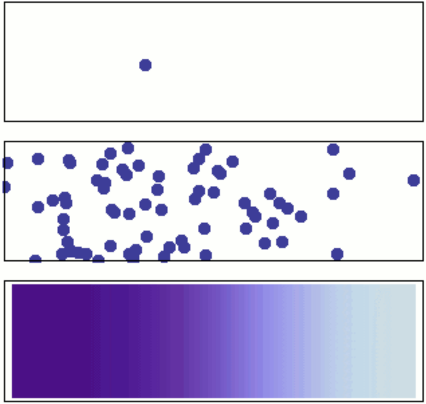


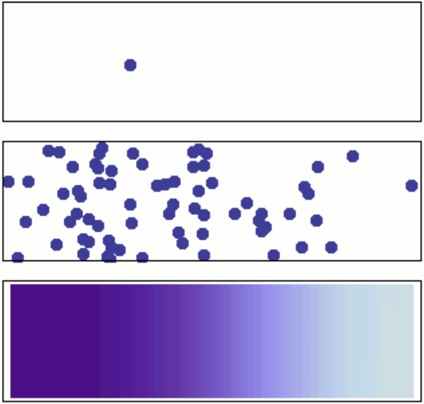


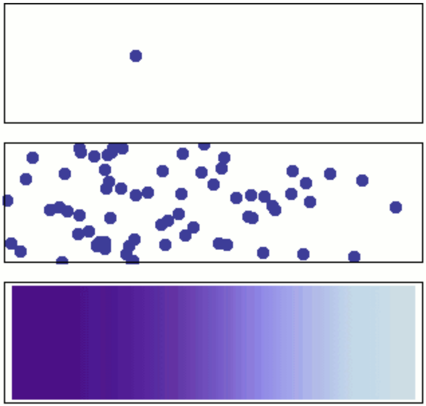


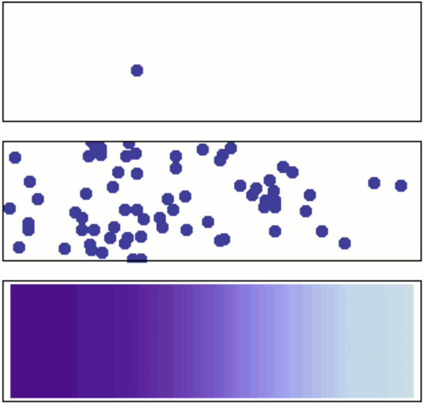


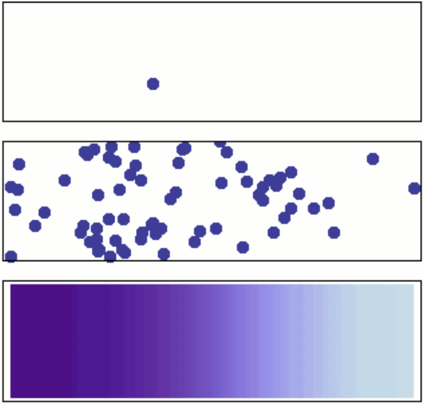


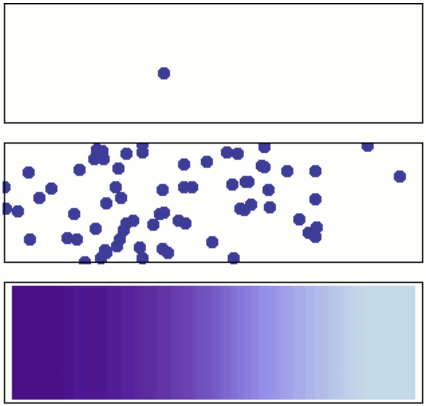


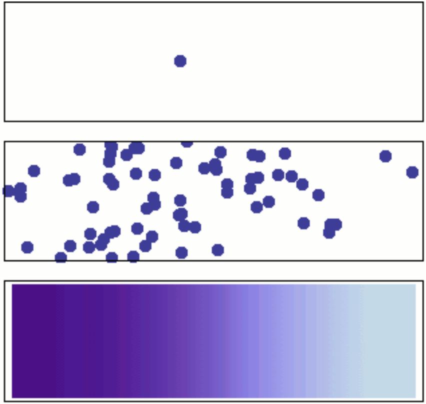


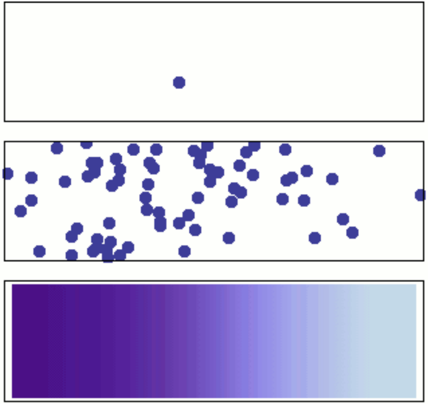


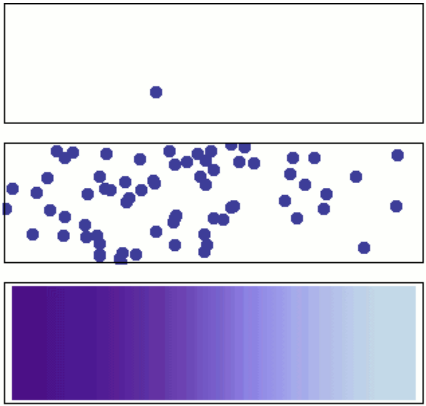


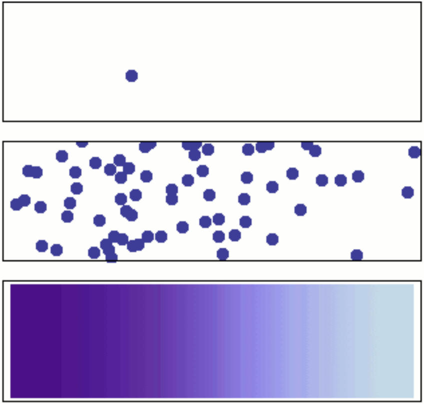


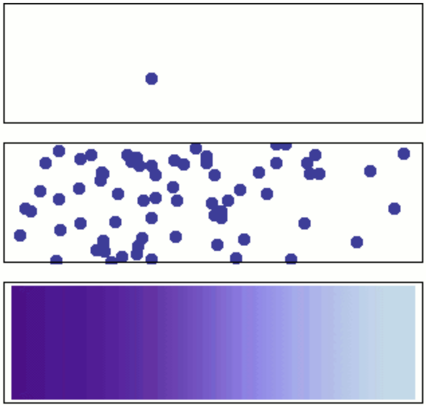


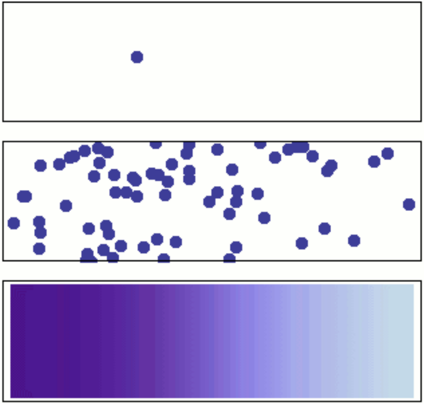


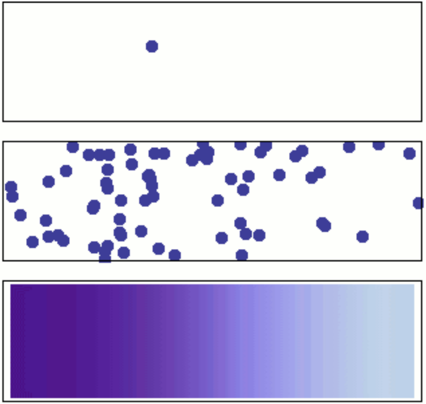


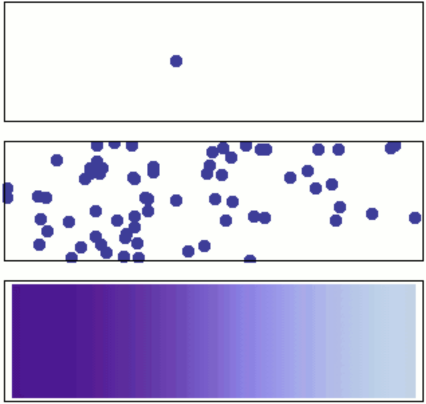


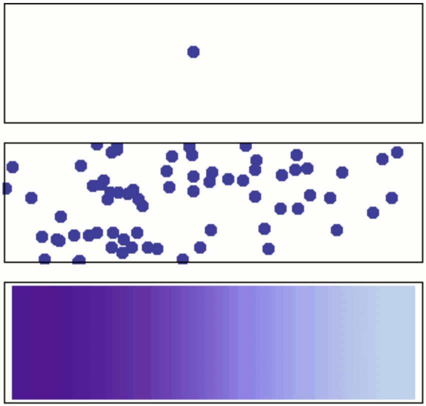


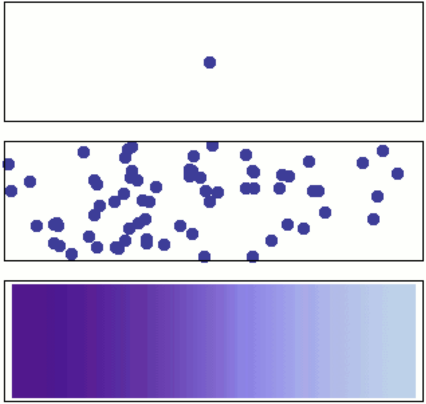


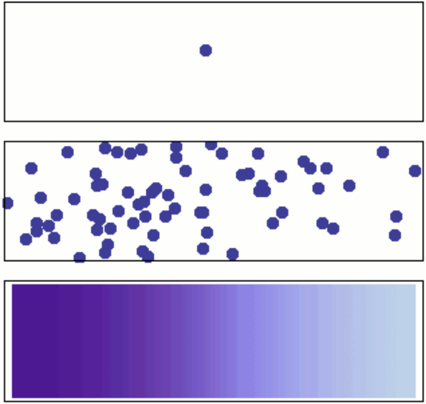


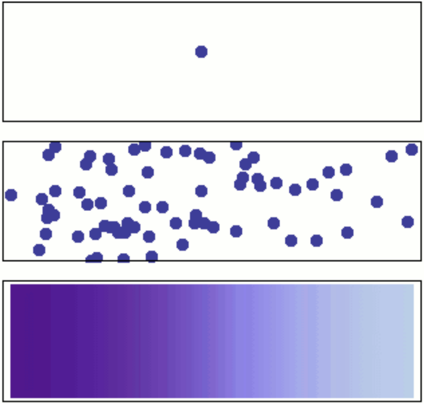


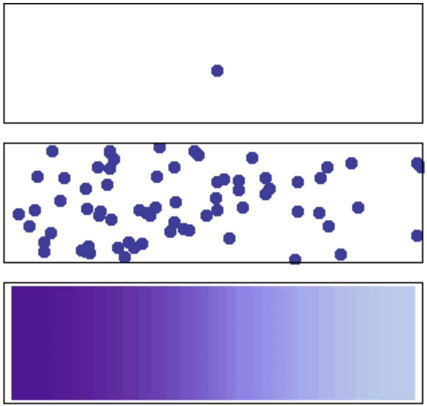


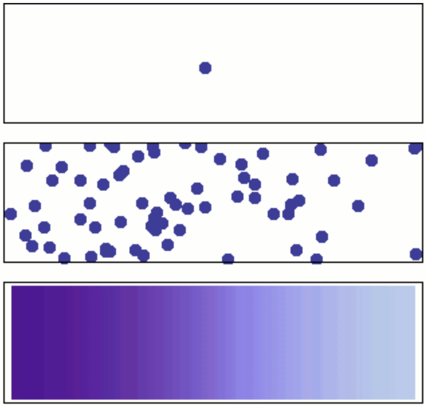


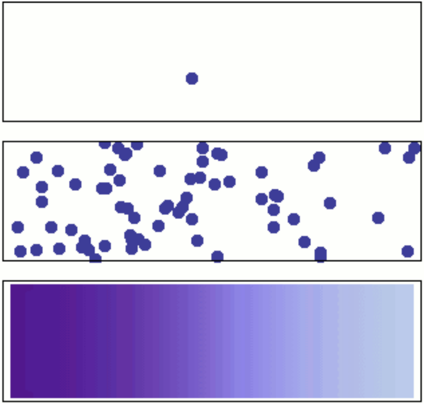


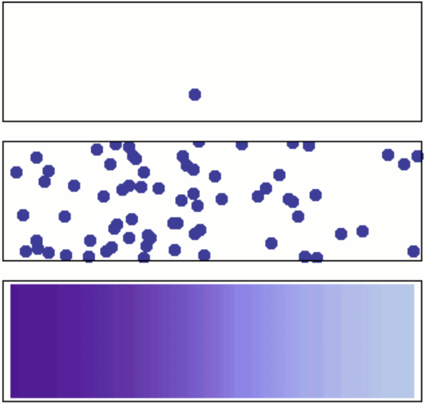


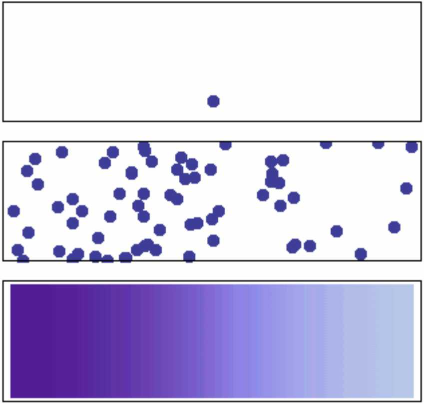


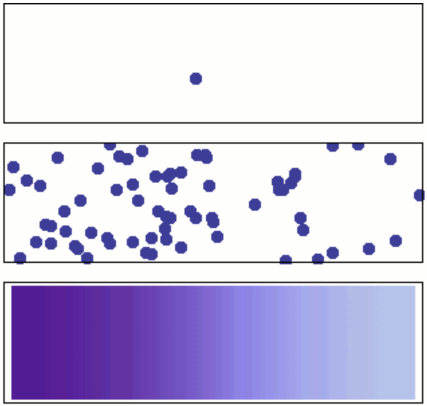


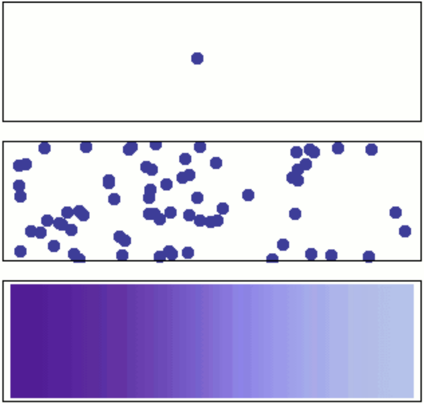


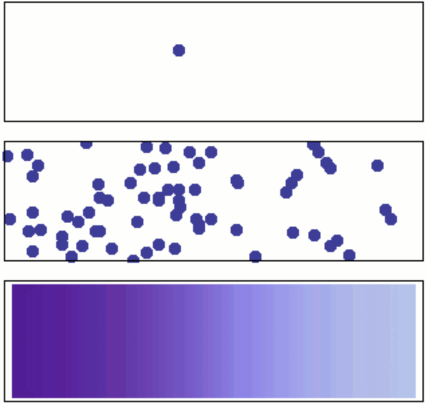


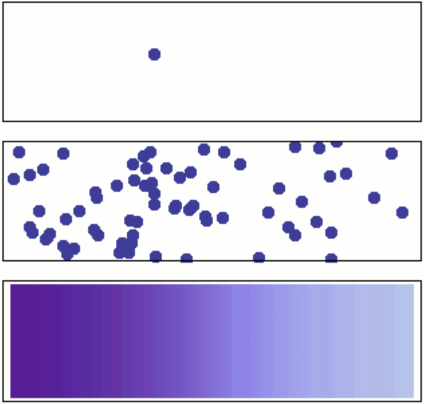


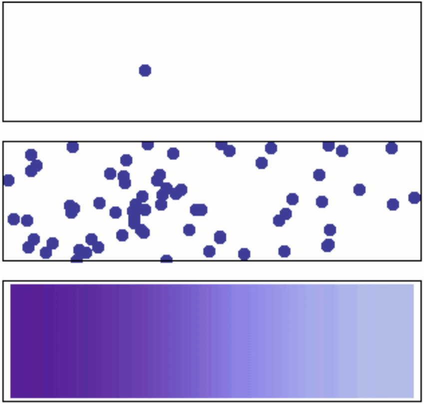


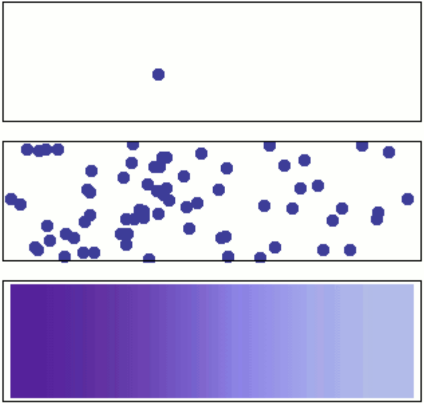


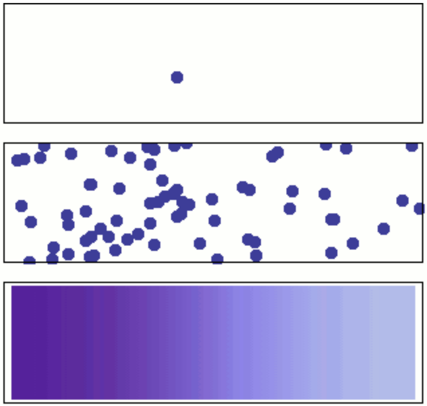


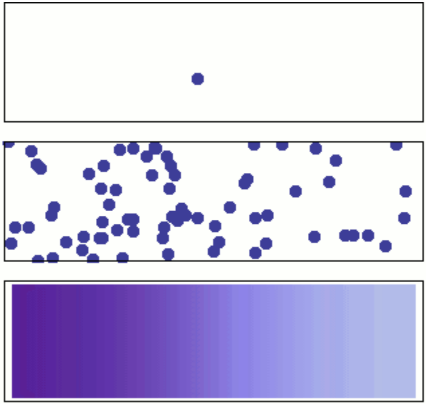


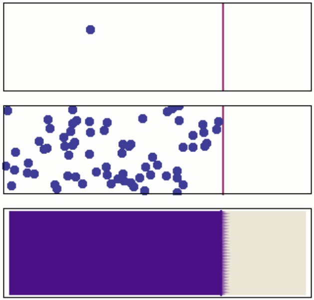












Fick's Law :

$$\begin{cases} \partial_t \rho(x,t) = \partial_x (D(\rho) \partial_x \rho(x,t)), \; t > 0, x \in [0,1] \\ \partial_x \rho(0,t) = \partial_x \rho(1,t) = 0, \quad t > 0 \end{cases}$$

Hamiltonian dynamics : two facts/objections

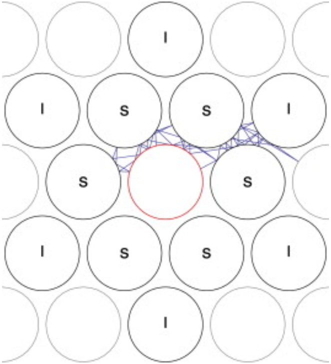
- Loschmidt : Microscopic dynamics is reversible, macroscopic dynamics is not.
- Zermelo : Hamiltonian dynamics in a bounded domain is almost surely recurrent.

Theorem : Poincaré recurrence theorem

Let $(X, \mathcal{A}, \mu)$ a measure space such that $\mu(X) < \infty$ and $f : X \to X$ a map such that for any $A \in \mathcal{A}$, $\mu(f^{-1}(A)) = \mu(A)$, then $\forall B \in \mathcal{A}$,

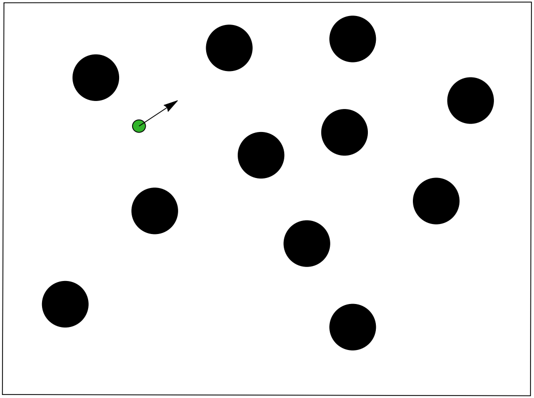
$$\mu[\{x \in B : \exists N, \forall n \geq N,\ f^n(x) \notin B\}] = 0$$

Periodic Lorentz gas

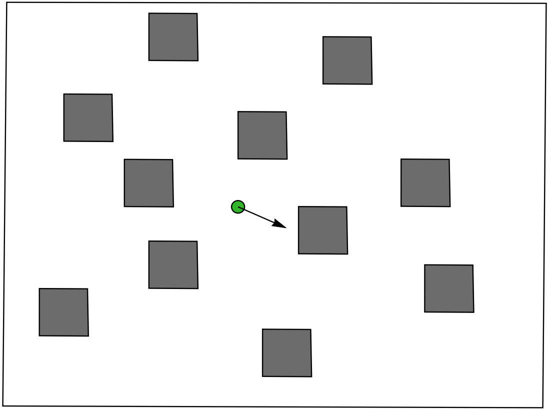


Bunimovich-Sinai shows that for large time the rescaled motion of a test particle is diffusive.

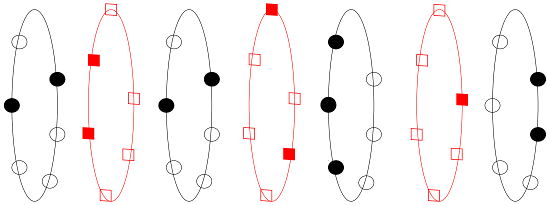
Random Lorentz gas

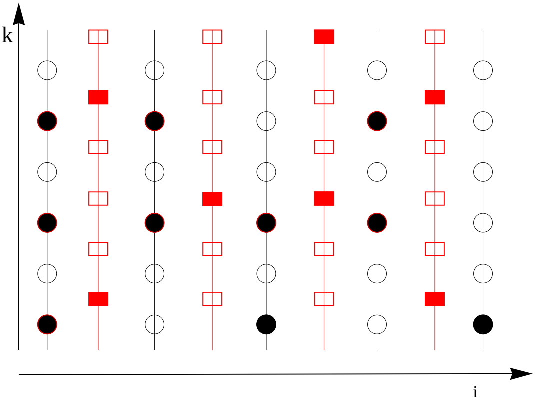


Ehrenfest random wind-tree model



The model

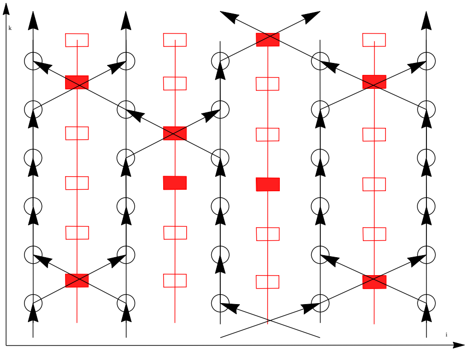




$$\mathcal{C}_N = \prod_{i \in \Lambda_N} \mathcal{R}_i = \{(k,i) : k \in \{1,\ldots,R\},\ i \in \{-N,\ldots,N\}\}.$$

Scatterers : variables $\xi(k,i) \in \{0,1\}$

The model



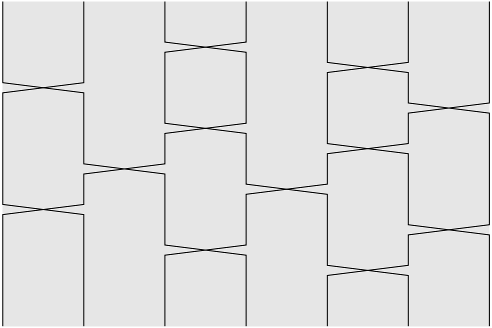
Dynamical system $\tau : \mathcal{C}_N \to \mathcal{C}_N$:

$$\begin{aligned} \tau(k,i) &= J(k,i)(k+1,i+1) + J(k,i-1)(k+1,i-1) \\ &+ (1-J(k,i))(1-J(k,i-1))(k+1,i) \end{aligned}$$

$$J(k,i) = \xi(k,i)(1-\xi(k,i-1))(1-\xi(k,i+1))$$

Balint Toth

- Graph $\Lambda = (\mathcal{V}, \mathcal{E})$.
- To each edge attach independent Poisson processes on $[0, \beta]$ of unit intensity, $\beta > 0$.
- For each realisations of the Poisson processes, create a set of "cycles".



Figures by Daniel Ueltschi !!

Other quantum spins systems : Aizenman-Nachtergaele's random loops.

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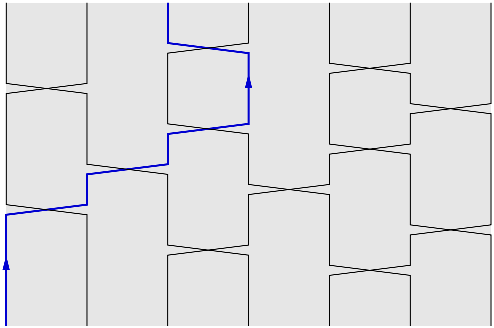

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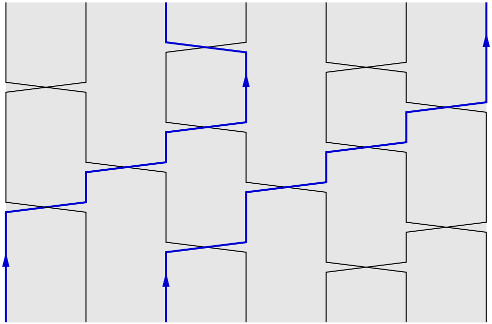

Figures by Daniel Ueltschi !!
Other quantum spins systems : Aizenman-Nachtergaele's random loops.

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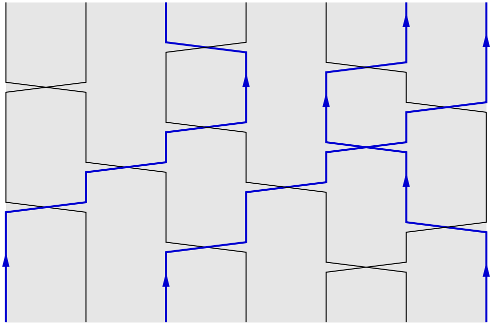

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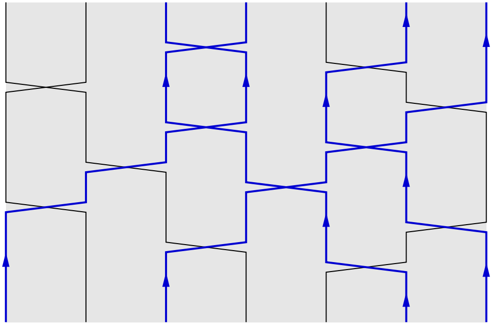

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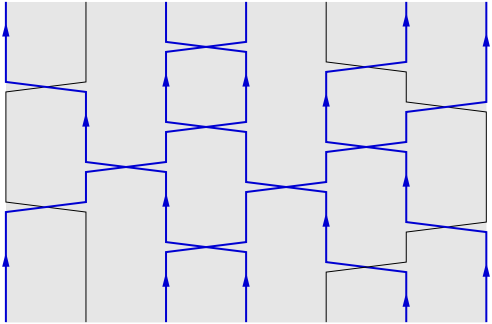

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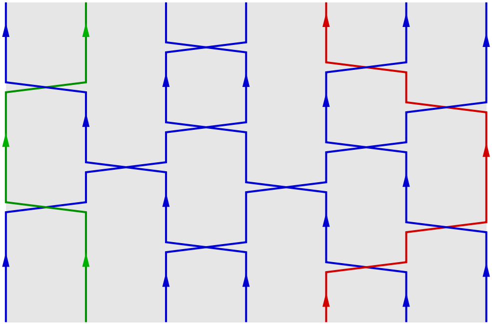

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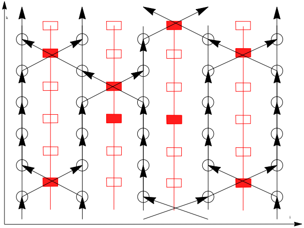
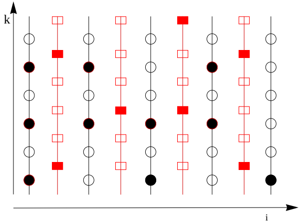
Evolution of occupation variables





Occupation variable of site $(k,i) \in \mathcal{C}_N$: $\sigma(k,i) \in \{0,1\}$. Evolution :

$$\sigma(k,i;t) = \sigma(\tau^{-t}(k,i);0), \ t \in \mathbb{N}^*$$

or recursion :

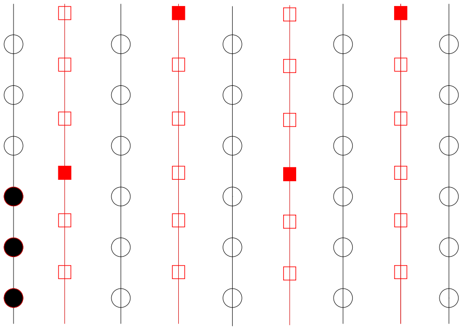
$$\begin{aligned}\sigma(k,i;t) &= (1 - J(k-1,i))(1 - J(k-1,i-1))\sigma(k-1,i;t-1) \\ &+ J(k-1,i-1)\sigma(k-1,i-1;t-1) + J(k-1,i)\sigma(k-1,i+1;t-1).\end{aligned}$$

$\sigma(\cdot;t)$ is permutation of initial occupation variables $\sigma(\cdot;0)$.

Facts

- Dynamics is *conservative*.
- τ is injective, thus *invertible* (reversible).
- Every point of $\mathcal{C}_N$ is *periodic* and $R \leq T(x) \leq R(2N+1), \quad \forall x \in \mathcal{C}_N$.

Interactions with no diffusion



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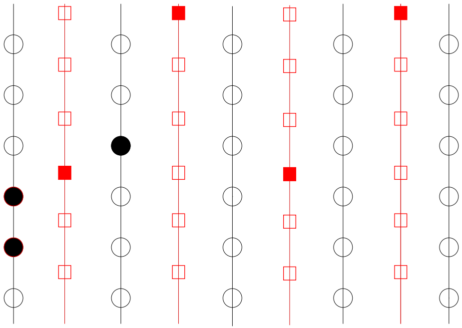

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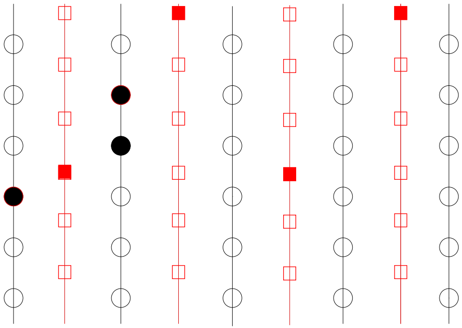

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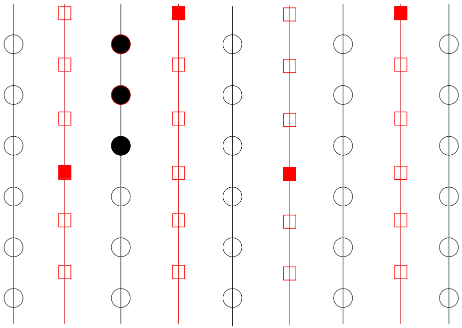

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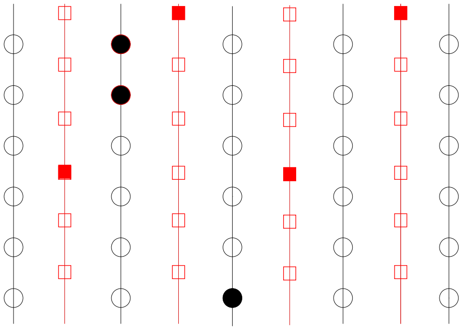

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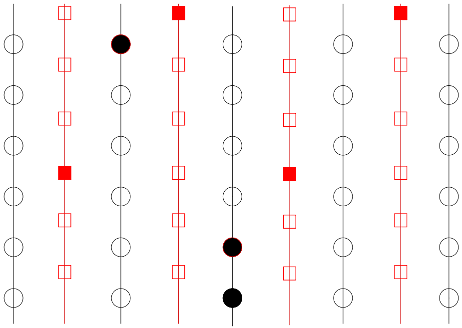

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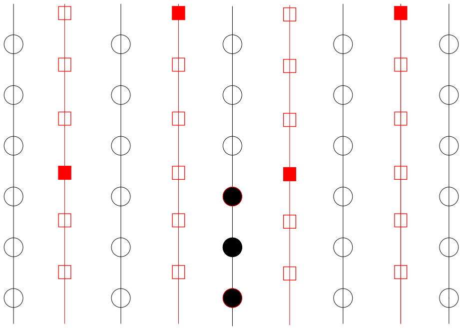

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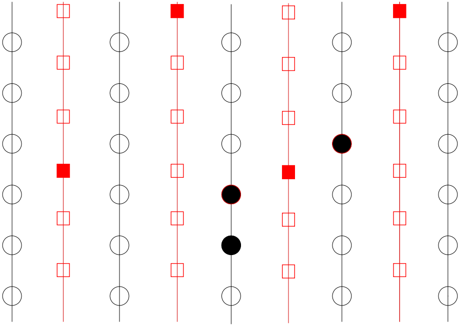

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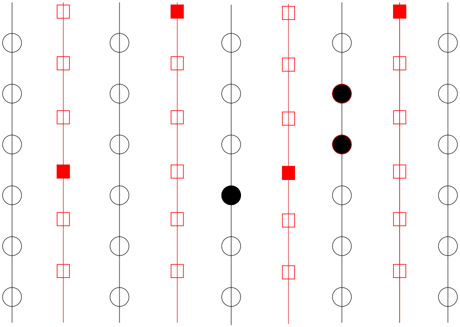
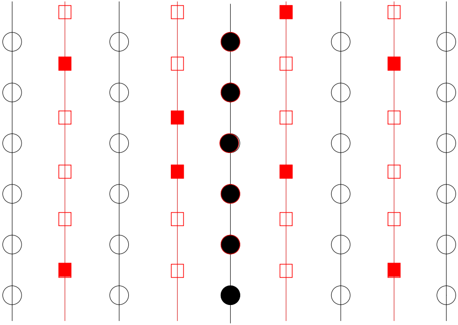


Diffusion



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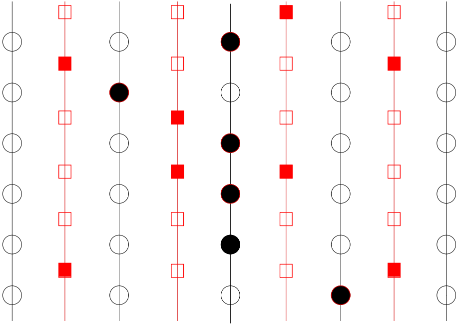

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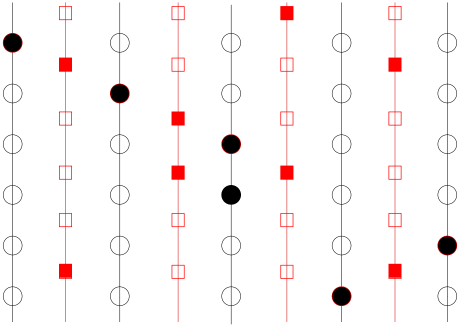

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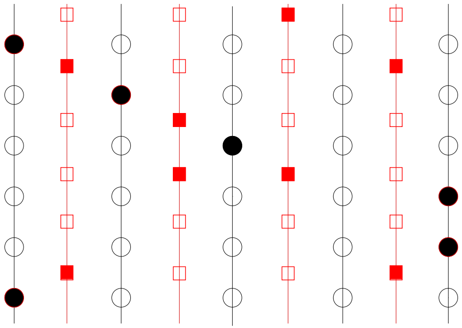

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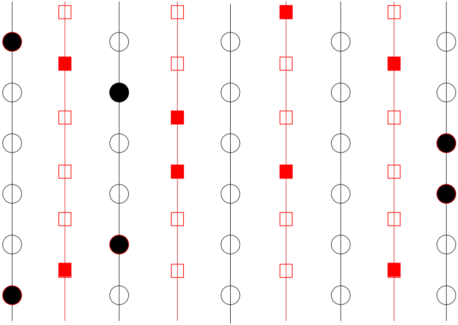

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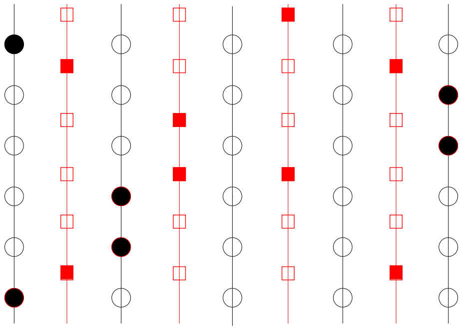

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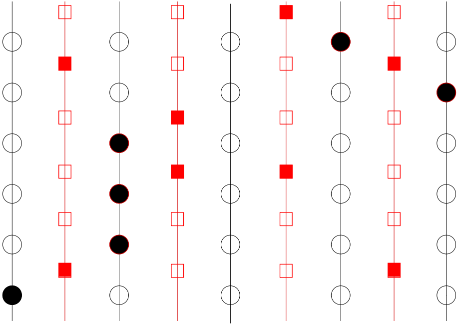

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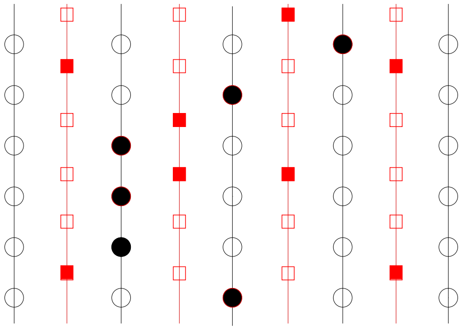

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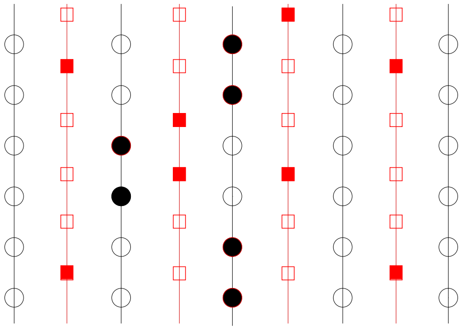


Macroscopic quantity of interest : *empirical density* of the rings

$$\rho^R(i,t) = \frac{1}{R} \sum_{k=1}^{R} \sigma(k,i,t)$$

- What's diffusion in this context ?
- For a given configuration of scatterers, does diffusion occur ?
- Sometimes yes, sometimes no.
- How often ?

Diffusion in discrete time and space

Let $0 < \mu < 1$, and the discrete time evolution system for $t \in \mathbb{N}$:

$$\begin{cases} \rho(i,t+1) = \rho(i,t) + \mu(1-\mu)^2 \left[\rho(i-1,t) + \rho(i+1,t) - 2\rho(i,t)\right] \\ \rho(-N,t+1) = \rho(-N,t) + \mu(1-\mu)[\rho(-N+1,t) - \rho(-N,t)] \\ \rho(N,t+1) = \rho(N,t) + \mu(1-\mu)[\rho(N-1,t) - \rho(N,t)] \end{cases}$$

Proposition

Let $\{h(i) > 0 : i \in \Lambda_N\}$ such that $\sum_{i\in\Lambda_N} h(i) = h$, and ρ_h such that $\rho_h(i) = \frac{h}{2N+1}$, $\forall i \in \Lambda_N$ then there exists a unique solution ρ such that

- $\rho(i,0) = h(i)$
- $\sum_{i\in\Lambda_N} \rho(i,t) = h$, $\forall t \in \mathbb{N}$.
- $\exists c > 0$ such that
$$\lim_{t\to\infty} e^{ct}||\rho(\cdot,t) - \rho_h|| = 0$$

Diffusion with high probability

Theorem

Let

- $\{\sigma(k,i;0) : (k,i) \in \mathcal{C}_N\}$ be a set of independent Bernoulli random variables such that $\mathbb{E}[\sigma(k,i,0)] = \hat{\rho}_i \in [0,1]\,, \forall k \in \{1,\ldots,R\}$
- $\{\xi(k,i) : (k,i) \in \mathcal{C}_N\}$ such that $\mathbb{E}[\xi(k,i)] = \mu \in]0,1[$.
- $\hat{\rho}(\cdot,t)$ be the solution of the above system with initial condition $\hat{\rho}(i,0) = \hat{\rho}_i$

then $\forall \epsilon > 0$ and $\forall \alpha \in]0,1[$,

$$\sup_{t\in[0,R^\alpha]} \mathbb{P}\left[\bigcup_{i=-N}^{N} \{|\rho^R(i,t) - \hat{\rho}(i,t)| > \epsilon\}\right] \leq \frac{C}{\epsilon^2 R^{1-\alpha}}.$$

If one chooses the configuration of scatterers as the result of independant heads and tails (with a bias given by μ), then as R goes to infinity, it is more and more unlikely to pick a configuration of scatterers that would lead to an evolution of the empirical densities that would be far from the reference solution $\hat{\rho}$ at any given time smaller than the minimal recurrence time.

Proof

Show :

$$\mathbb{E}[\rho^R(i,t)] = \hat{\rho}(i,t),\ i \in \Lambda_N,\ 0 < t < R^\alpha.$$

Use

- $$\begin{aligned}\sigma(k,i;t) &= (1-J(k-1,i))(1-J(k-1,i-1))\sigma(k-1,i;t-1) \\ &+ J(k-1,i-1)\sigma(k-1,i-1;t-1) + J(k-1,i)\sigma(k-1,i+1;t-1).\end{aligned}$$
- $J(k-1,i)J(k-1,i-1) = 0$
- $\mathbb{E}[J(k-1,i)] = \mathbb{E}[J(k-1,i-1)] = \mu(1-\mu)^2,\ \forall\, 1 \le k \le R,$
- *Independance* between $\sigma(k-1,i,t-1)$ and the scatterer "ahead" for $t < R^\alpha < R$.

$$\mathbb{E}[\rho^R(i,t)] - \mathbb{E}[\rho^R(i,t-1)] = \mu(1-\mu)^2 \left(\mathbb{E}[\rho^R(i-1,t-1)] + \mathbb{E}[\rho^R(i+1,t-1) - 2\mathbb{E}[\rho^R(i,t-1)]\right)$$

Same than diffusion equation.

Proof

Next, bound variance of the macroscopic density :

$$\begin{aligned}\mathrm{Var}[\rho^R(i,t)] &= \frac{1}{R^2}\mathbb{E}[\left(\sum_{k=1}^{R}\sigma(k,i;t) - \sum_{k=1}^{R}\mathbb{E}[\sigma(k,i;t)]\right)^2] \\ &= \frac{1}{R^2}\left(\mathbb{E}[\sum_{k,k'=1}^{R}\sigma(k,i;t)\sigma(k',i;t)] - (\sum_{k=1}^{R}\mathbb{E}[\sigma(k,i;t)])^2\right)\end{aligned}$$

Proof

Remember $\sigma(k,i;t) = \sigma(\tau^{-t}(k,i);0)$, then

$$\mathbb{E}[\sigma(k,i;t)] = \sum_{x \in \mathcal{C}_N} \mathbb{E}[\sigma(x;0)]\mathbb{P}[\tau^{-t}(k,i) = x]$$

$$\mathbb{E}[\sigma(k,i;t)\sigma(k',i;t)] = \sum_{x,x' \in \mathcal{C}_N} \mathbb{E}[\sigma(x;0)\sigma(x';0)]\mathbb{P}[\tau^{-t}(k,i) = x, \tau^{-t}(k',i) = x'].$$

When $k \neq k'$, we get :

$$\mathbb{E}[\sigma(k,i;t)\sigma(k',i;t)] = \sum_{x \neq x' \in \mathcal{C}_N} \mathbb{E}[\sigma(x;0)]\mathbb{E}[\sigma(x';0)]\mathbb{P}[\tau^{-t}(k,i) = x, \tau^{-t}(k',i) = x']$$

because

- If $k \neq k'$, then $\tau^{-t}(k,i) \neq \tau^{-t}(k',i)$
- Initial occupation variables are *independent*.

Proof

$$\mathrm{Var}[\rho^R(i,t)] \leq \frac{1}{R} + \frac{1}{2R^2} \Big| \sum_{k \neq k'} \sum_{x,x' \in \mathcal{C}_N} \mathbb{E}[\sigma(x;0)]\mathbb{E}[\sigma(x';0)]\Delta[(k,x),(k',x');t] \Big|$$

where

$$\Delta[(k,x),(k',x');t] = \mathbb{P}[\tau^{-t}(k,i) = x, \tau^{-t}(k',i) = x'] - \mathbb{P}[\tau^{-t}(k,i) = x]\mathbb{P}[\tau^{-t}(k',i) = x']$$

By rotational invariance :

$$\mathrm{Var}[\rho^R(i,t)] \leq \frac{1}{R} + \frac{1}{R} \Big| \sum_{k' \neq 1} \sum_{x,x' \in \mathcal{C}_N} \mathbb{E}[\sigma(x;0)]\mathbb{E}[\sigma(x';0)]\Delta[(1,x),(k',x');t] \Big|.$$

If $t+1 < k' \leq R-t+1$ then $\tau^{-t}(1,i)$ and $\tau^{-t}(k',i)$ are independent random variables and for those k',

$$\Delta[(1,x),(k',x');t] = 0.$$

Proof

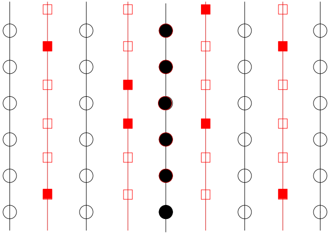
$$
\begin{aligned}
\mathrm{Var}[\rho^R(i,t)] \leq\ & \frac{1}{R} + \frac{1}{R} \sum_{\substack{R-t+1<k'\leq R \\ 1<k'\leq t+1}} \sum_{x,x'\in\mathcal{C}_N} \mathbb{P}[\tau^{-t}(1,i)=x, \tau^{-t}(k',i)=x'] \\
+\ & \frac{1}{R} \sum_{\substack{R-t+1<k'\leq R \\ 1<k'\leq t+1}} \sum_{x,x'\in\mathcal{C}_N} \mathbb{P}[\tau^{-t}(1,i)=x]\mathbb{P}[\tau^{-t}(k',i)=x'] \\
\leq\ & \frac{1}{R} + \frac{4(t-1)}{R} \\
\leq\ & \frac{6}{R^{1-\alpha}}, \text{for } R \text{ large enough.}
\end{aligned}
$$

Questions

Carlos Mejia-Monasterio (Madrid), Justin Salez (Paris Diderot), Daniel Ueltschi (Warwick)

- Go to higher dimension
- Take $R \sim N$ and take hydrodynamic limit to obtain "continuous" diffusion equation
- Properties of the stationary state
- Large deviations, entropy
- Relate Fick's law to crossing probabilities
- Distribution of periods

Distribution of the periods



$$T(k,i) = \inf\{n : \tau^n(k,i) = (k,i)\}$$

$$T(k,i) \in \{R, 2R, \ldots, (2N+1)R\}$$

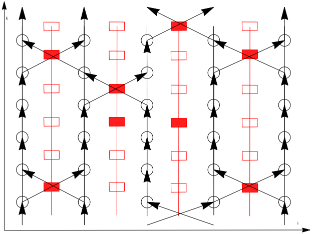
Question

Compute $\mathbb{P}[T(k,i) = lR]$, $\forall l \in \{1, 2, \ldots, (2N+1)\}$

Define a new map $\hat{\tau} : \Lambda_N \to \Lambda_N$ by

$$\hat{\tau}(i) = h(\tau^R(1,i)), \quad \forall i \in \Lambda_N$$

h is the projection : $h(k,i) := i$, $\forall (k,i) \in \mathcal{C}_N$



Distribution of the periods

Proposition

$\hat{\tau}$ is a random permutation such that $\hat{\tau} = \lambda_R \circ \ldots \circ \lambda_1$ where $(\lambda_i)_{1 \leq i \leq R}$ are i.i.d random permutations having same law than the permutation λ defined by

$$\lambda(i) \quad = (i+1)J(i) + (i-1)J(i-1) + i(1 - J(i))(1 - J(i-1)), \quad i \in \Lambda_N$$

where

$$J(i) = \xi(i)(1 - \xi(i-1))(1 - \xi(i+1)), \quad \xi(i) \sim \mathrm{Ber}(\mu), \quad \xi(-N-1) = \xi(N) = 0$$

One can define the length of a cycle containing $i \in \Lambda_N$,

$$\hat{T}(i) = \inf\{n : \hat{\tau}^n(i) = i\}$$

and we have :

$$\mathbb{P}[T(1,i) = nR] = \mathbb{P}[\hat{T}(i) = n].$$

Distribution of the periods

The distribution of the length of the cycles of random permutations (card shufflings) of N objects have been extensively studied.

- If the law of the permutation is uniform the distribution of the length of the cycles is uniform
- Yuval Peres : convergence (total variation) with cutoff $N^3 \log N$ of the adjacent random transposition to the uniform permutation

Simulation :