Diffusion in a random lattice Lorentz gas

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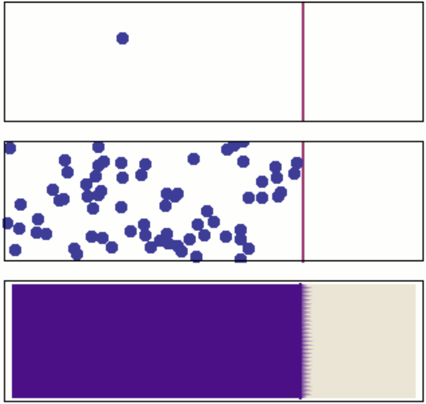
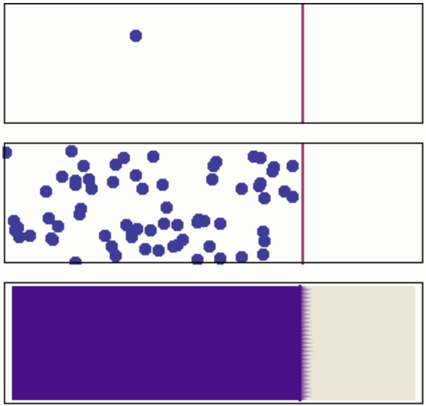
Goal: Introduce a new model designed to derive macroscopic diffusion from a deterministic (but with random parameters) microscopic dynamics in a "'typical" sense.

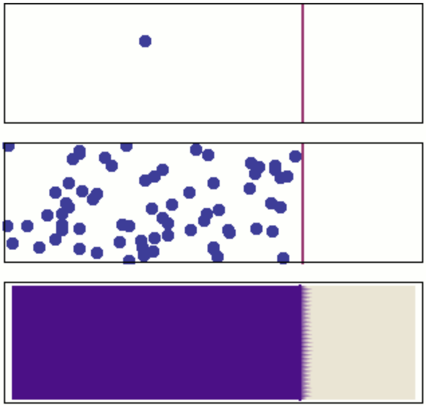
R. Lefevere *Macroscopic diffusion from a Hamilton-like dynamics* Journal of Statistical Physics, Volume 151 (5),861-869 (2013)

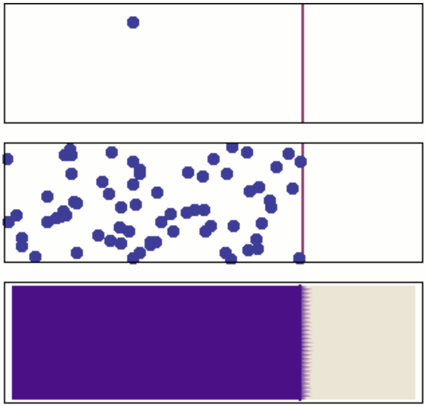
R. Lefevere *Fick's law in a random lattice Lorentz gas* arXiv:1404.5694 to appear in Archive for Rational Mechanics and Analysis

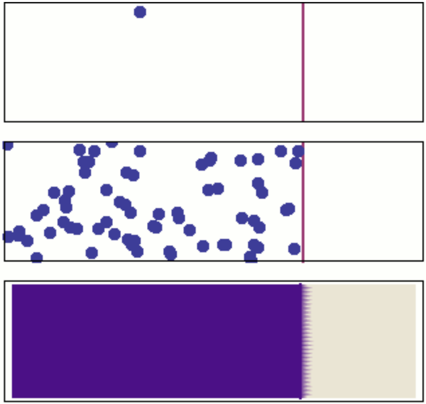
Diffusion of particles : Fick's law

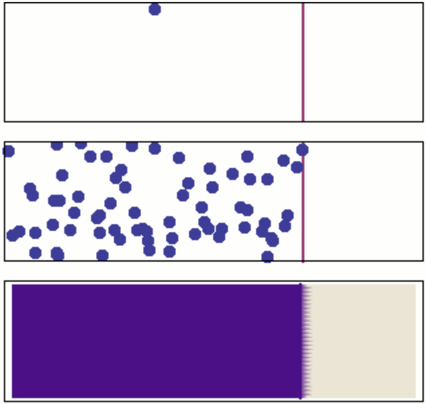


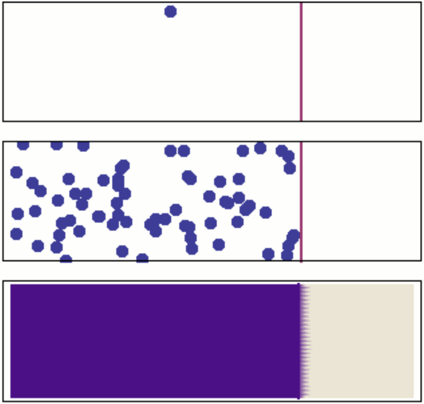


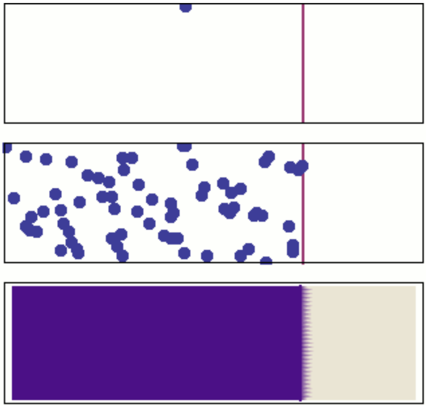


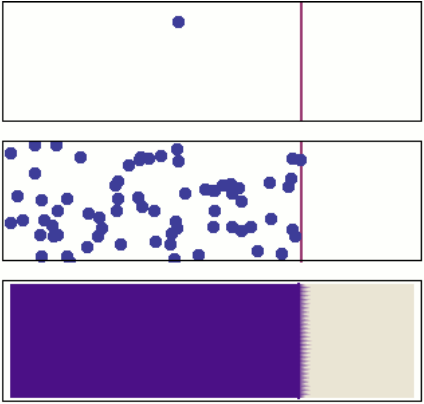


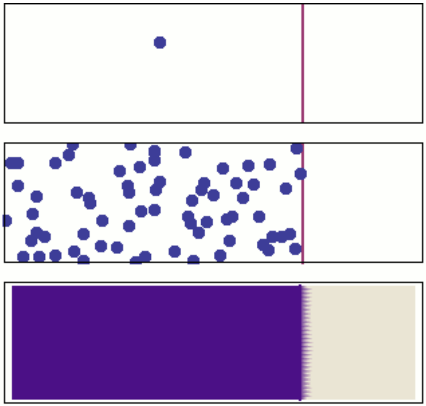


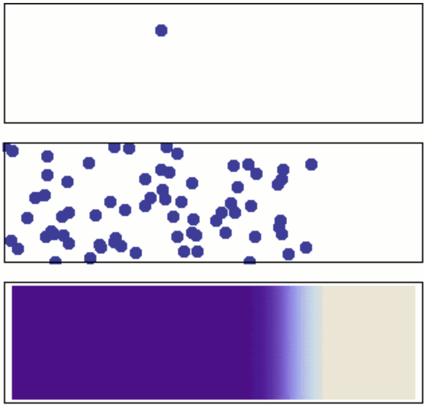


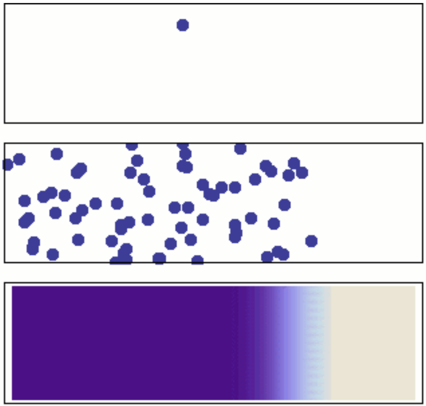


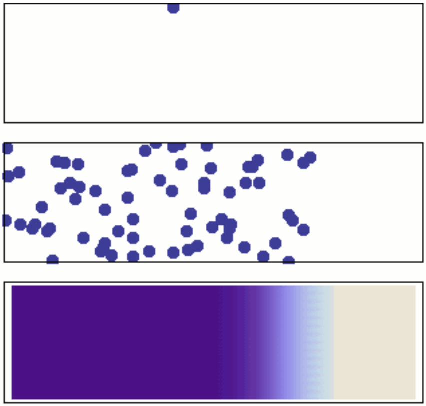


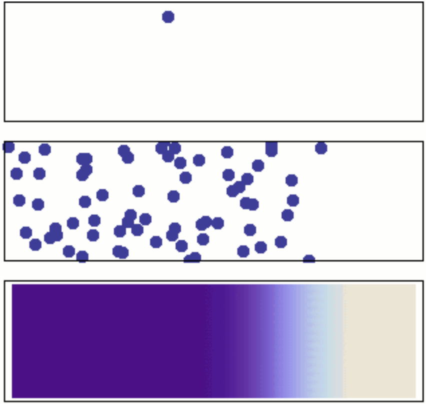


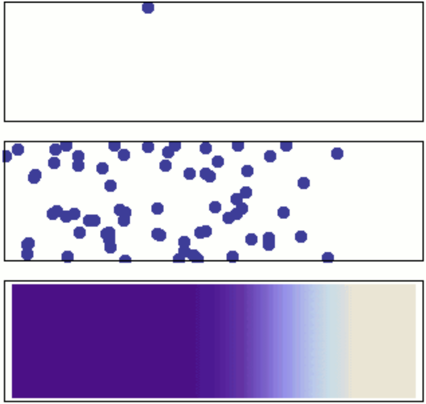


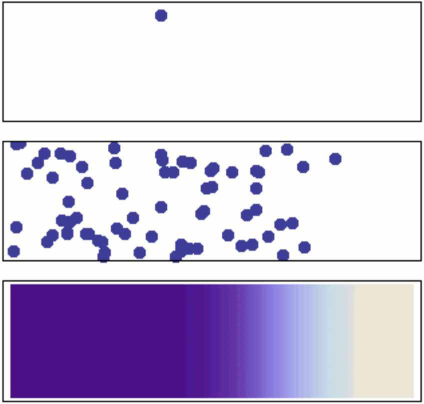


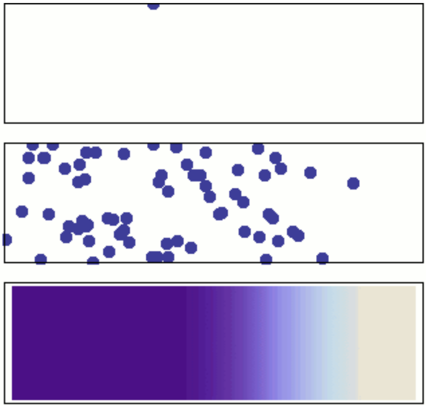


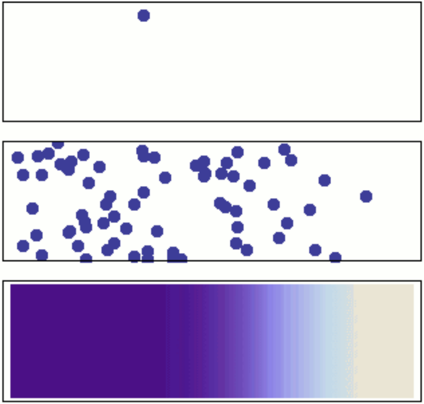


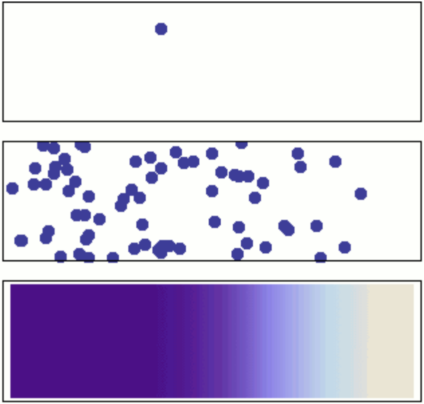


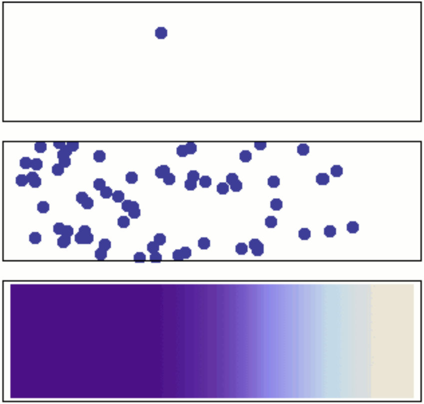


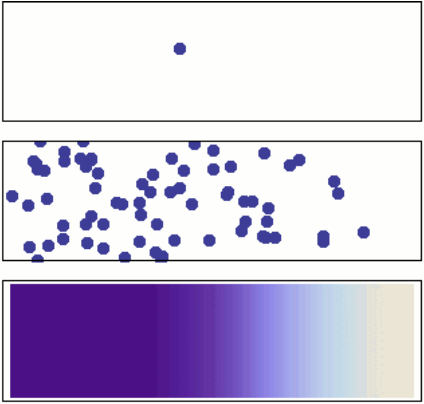


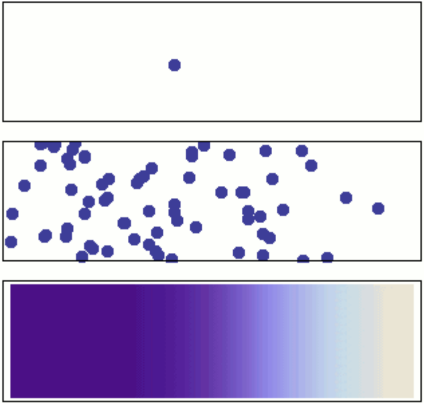


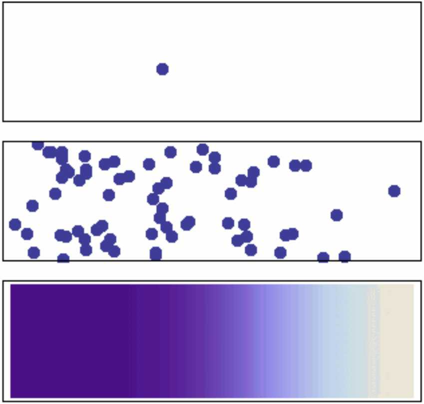


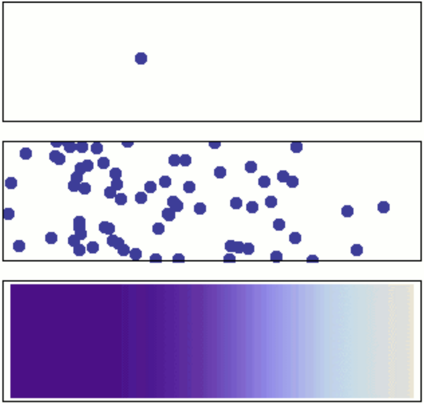


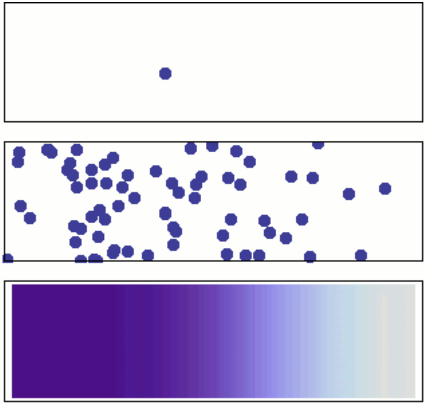


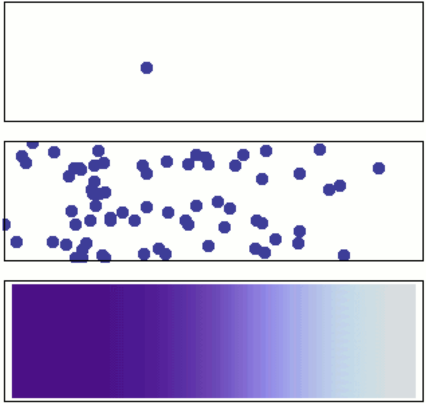


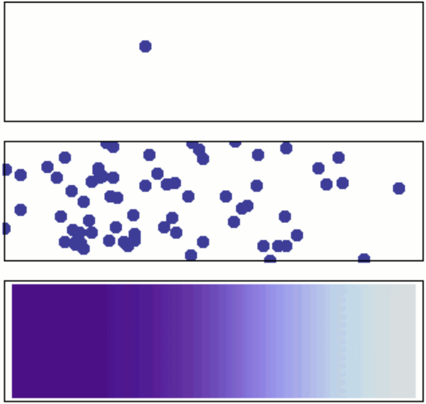


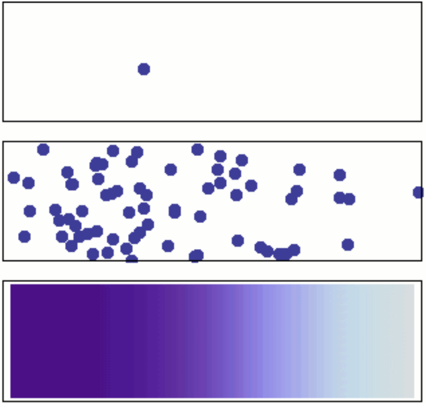


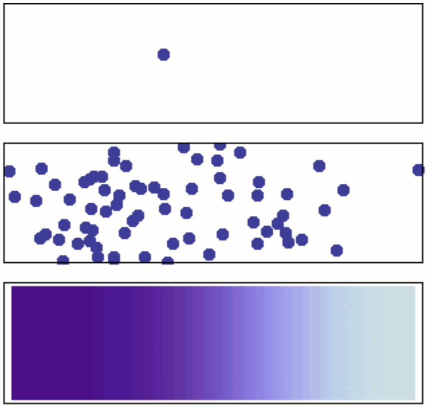


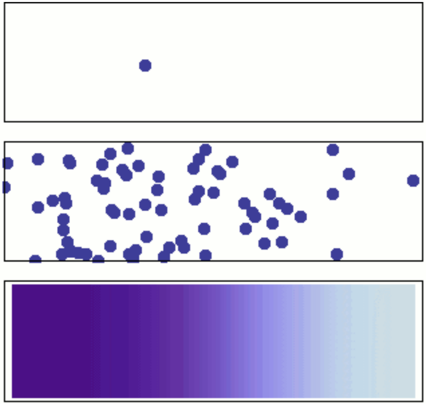


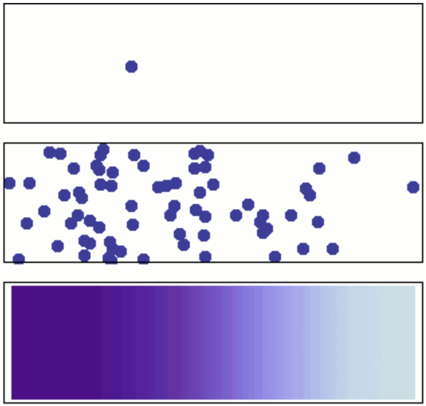


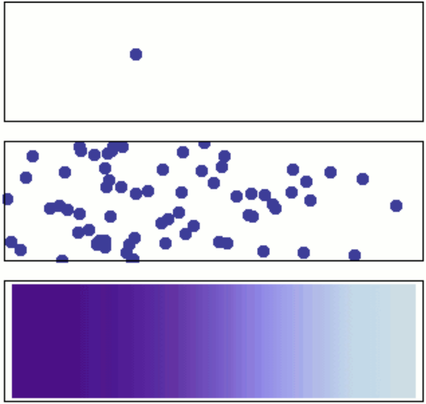


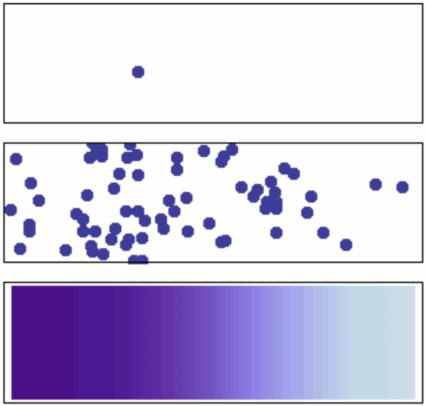


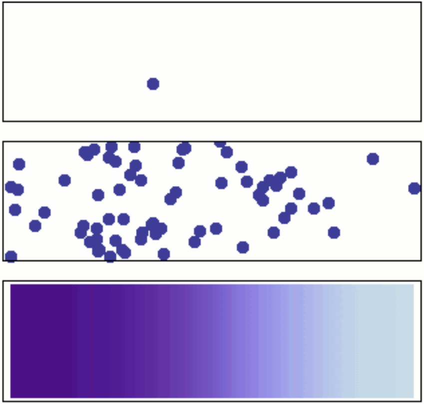


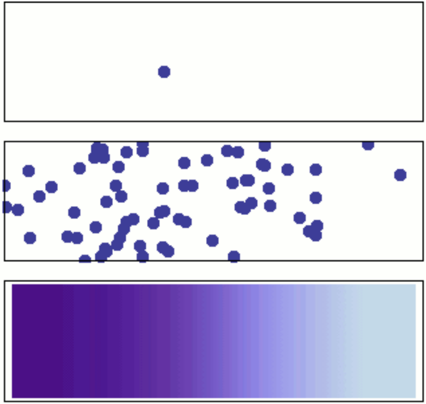


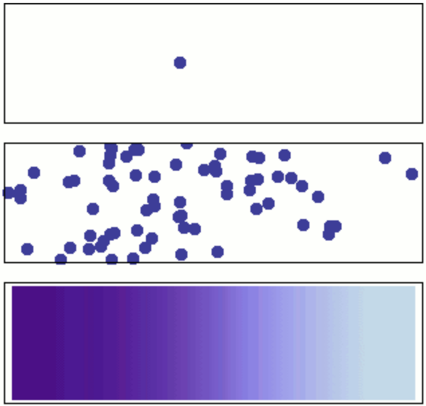


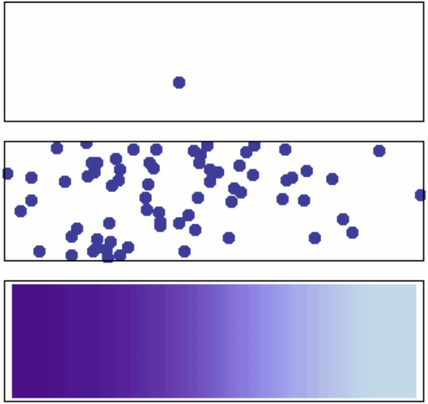


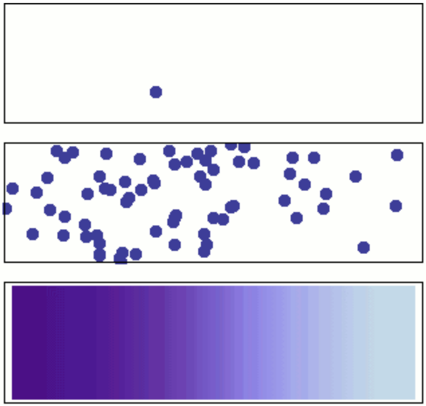


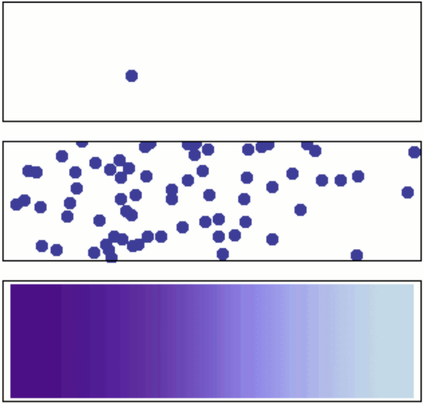


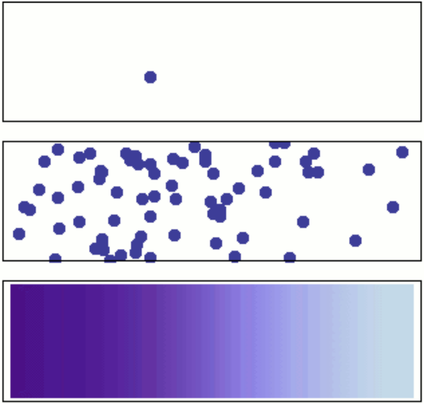


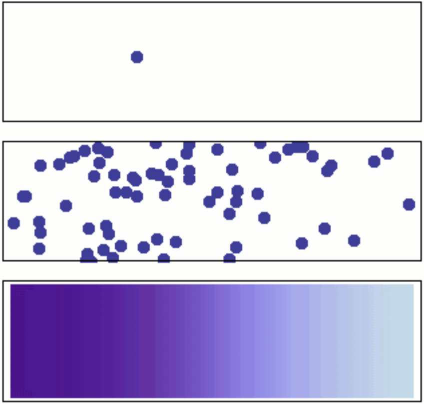


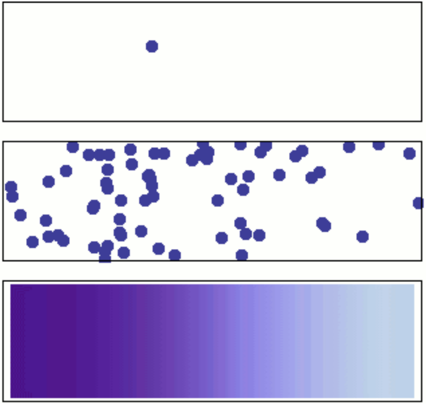


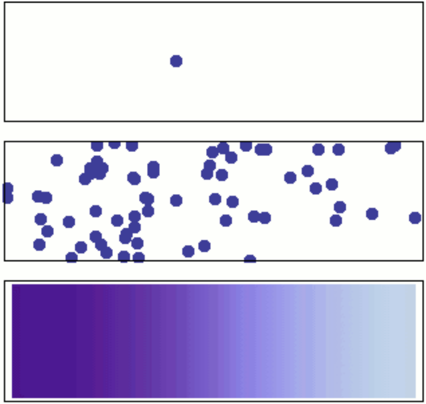


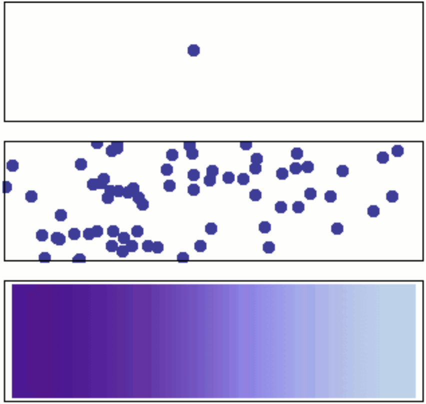


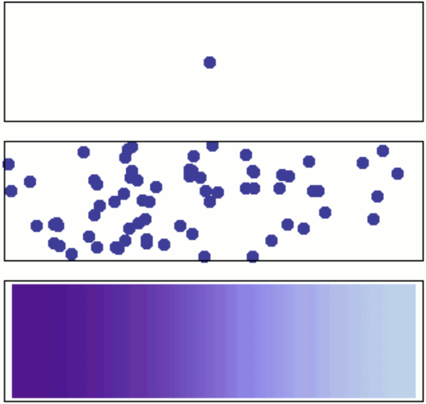


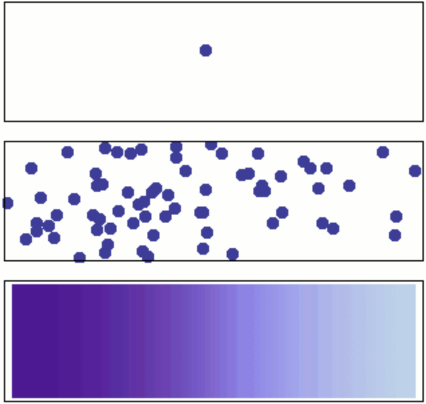


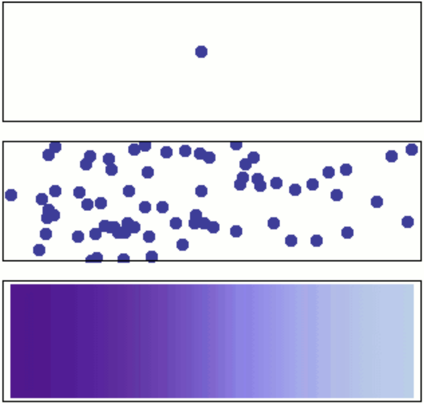


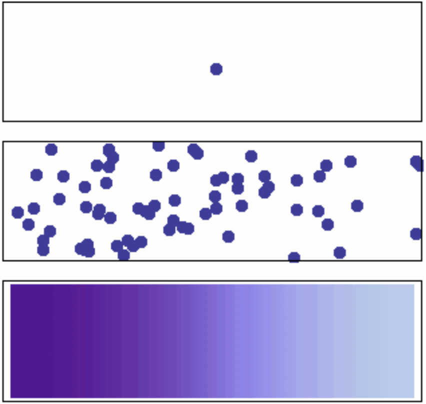


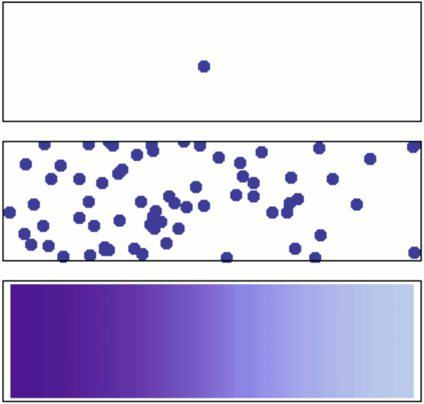


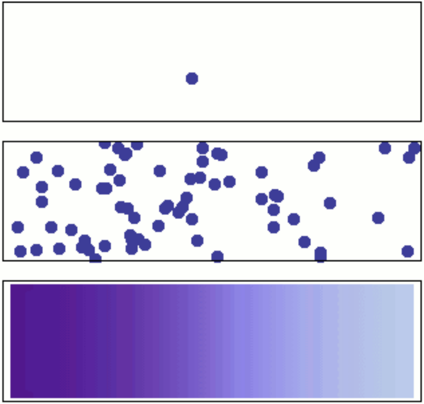


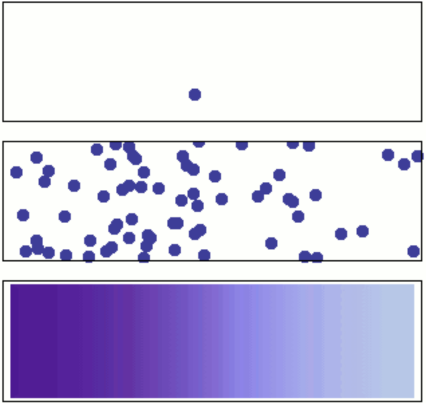


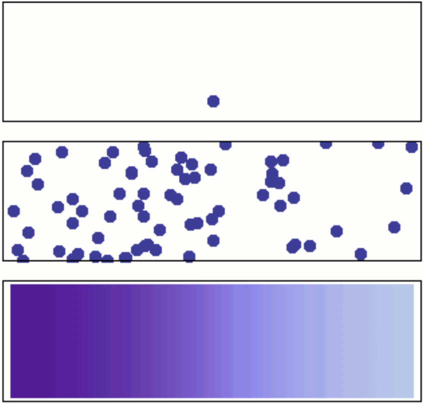


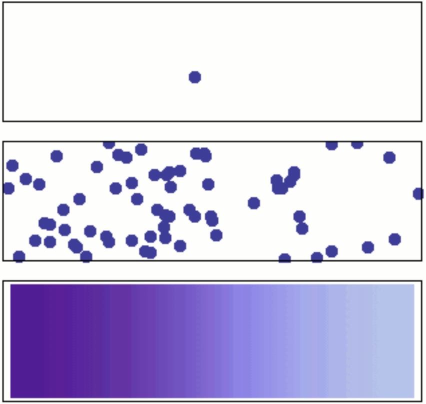


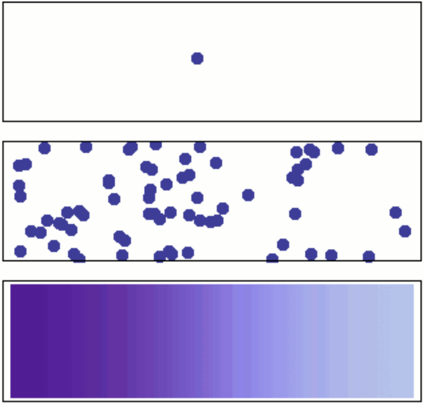


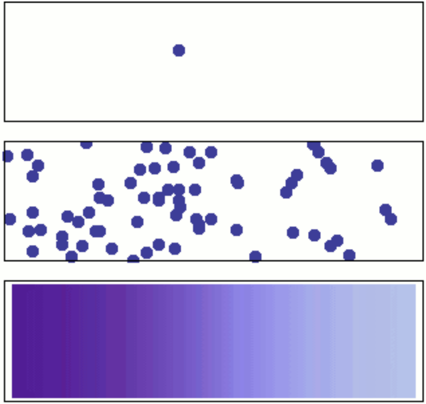


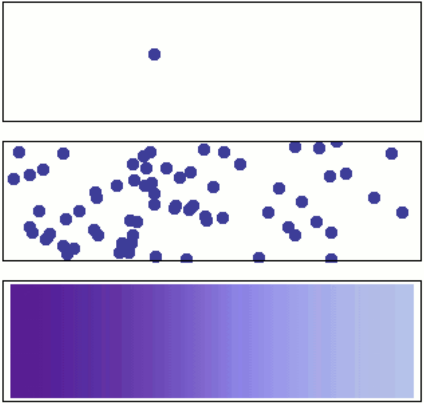


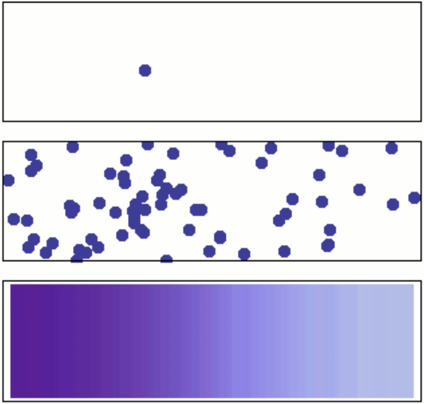


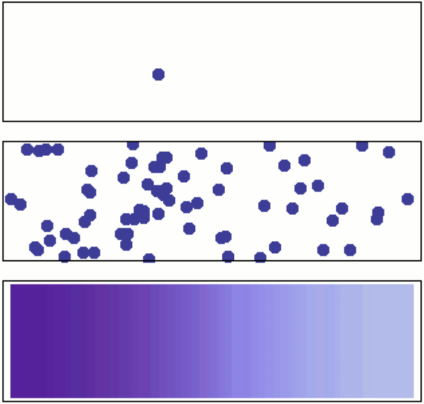


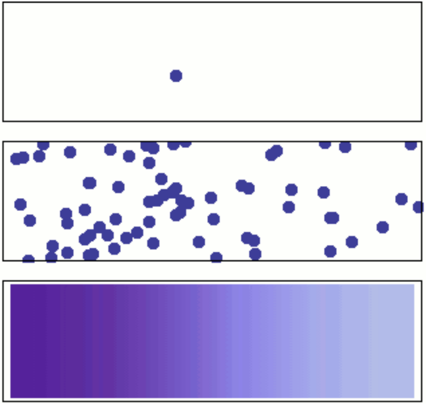


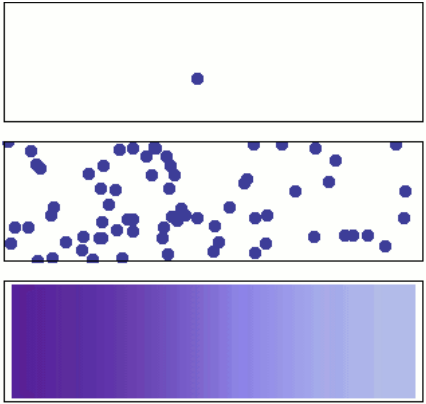


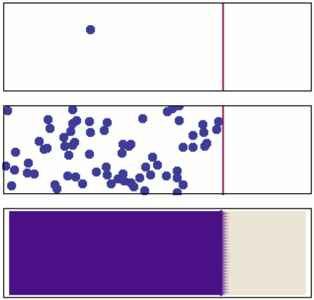












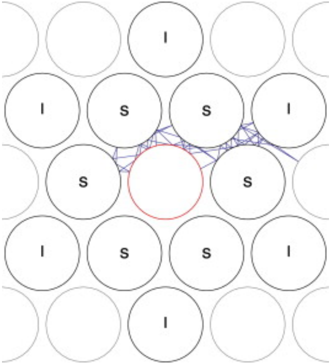
Look at the problem with particles reservoirs at the boundaries :

$$\begin{cases} \partial_t \rho(x,t) = -\partial_x j(x,t), \ t>0, x \in [0,L] \\ j(x,t) = -\kappa(\rho(x,t))\partial_x \rho(x,t) \\ \rho(0,t) = \rho_-, \ \rho(L,t) = \rho_+, \quad t>0 \\ \rho(x,0) = \rho^I(x) \end{cases}$$

If $\kappa(\rho) = \kappa$, then (exponentially fast) as $t \to \infty$, $\rho(x,t)$ and $j(x,t)$ approach

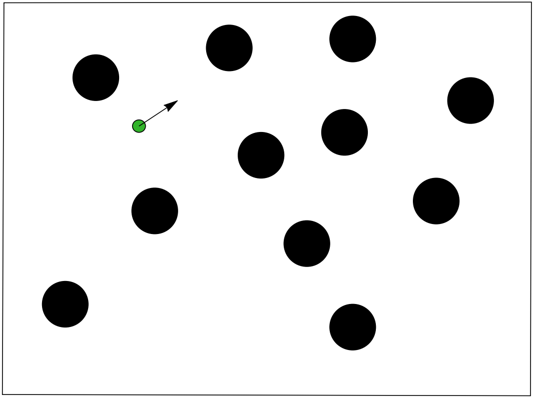
$$\begin{cases} \rho(x) = \rho_-(1-\frac{x}{L}) + \frac{x}{L}\rho_+ \\ j(x) = \frac{\kappa}{L}(\rho_+ - \rho_-) \end{cases}$$

Periodic Lorentz gas

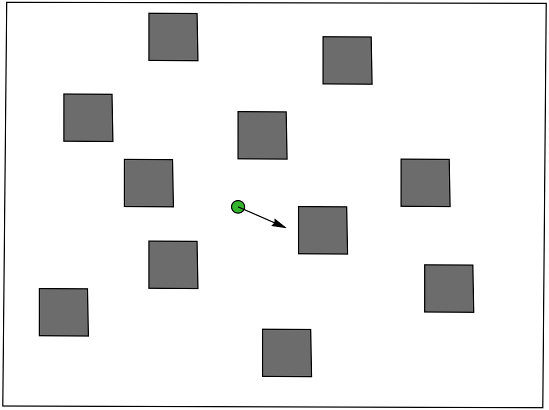


Bunimovich-Sinai shows that for large time the rescaled motion of a test particle is diffusive.

Random Lorentz gas



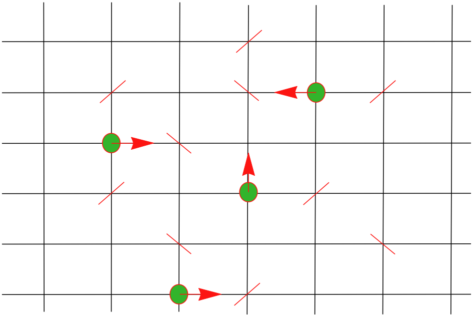
Ehrenfest random wind-tree model



Mirrors model

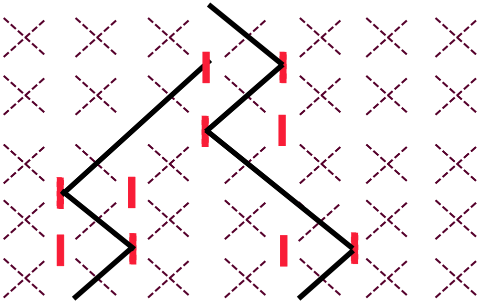
Ruijgrok-Cohen(1990,1991), Bunimovich :Deterministic walk in random environment

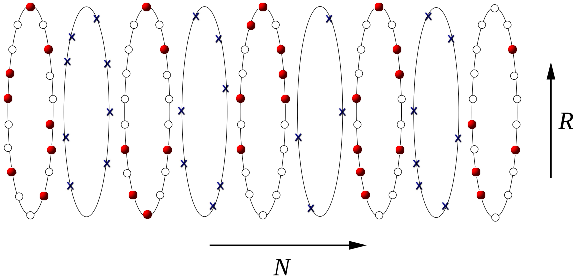
Mirrors model



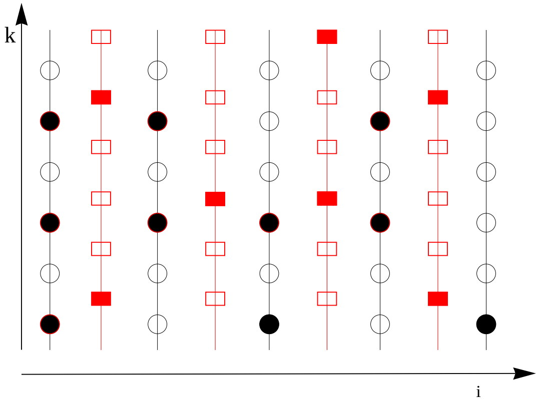
- System of size N
- Coupling on boundaries to particle reservoirs
- Current of particles J_N in the stationary state

Mirrors model



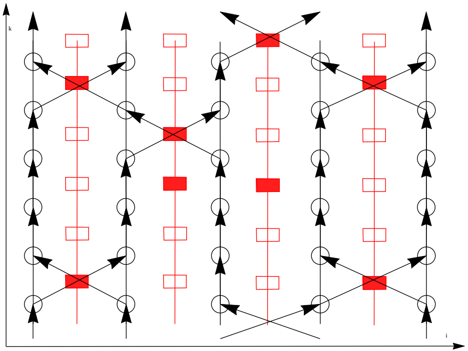

R
N

The model



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

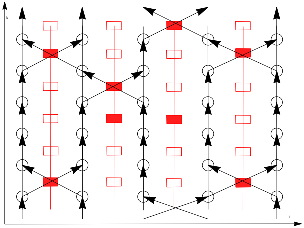
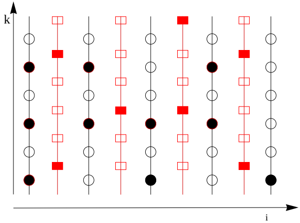
Scatterers : variables $\xi(k,i) \in \{0,1\}$



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

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

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

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

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

or recursion :

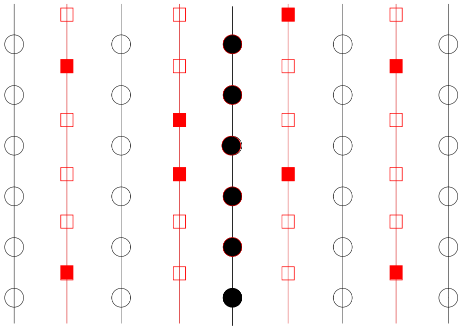
$$\begin{aligned}\sigma(k,i;t) &= (1-c(k-1,i))(1-c(k-1,i-1))\sigma(k-1,i;t-1)\\ &+ c(k-1,i-1)\sigma(k-1,i-1;t-1) + c(k-1,i)\sigma(k-1,i+1;t-1).\end{aligned}$$

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

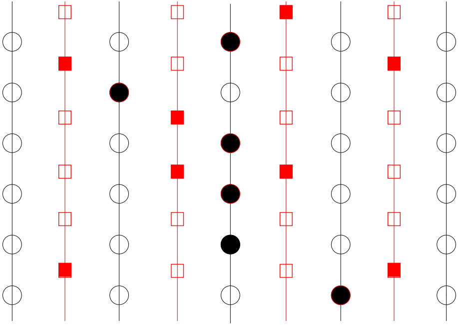
Facts

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

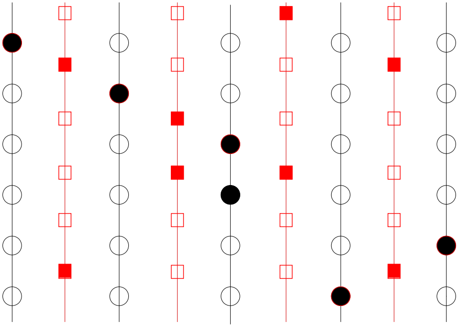
Diffusion



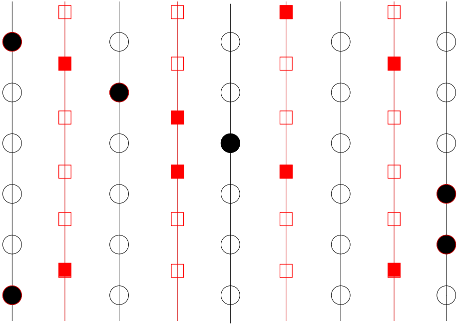
Diffusion



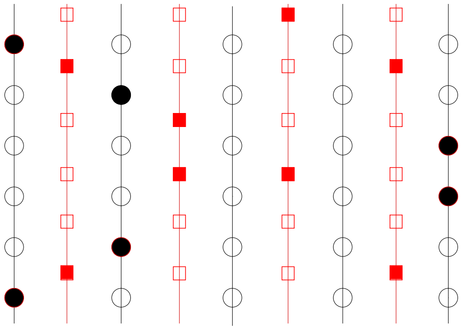
Diffusion



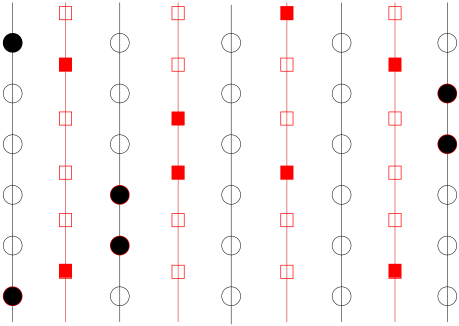
Diffusion



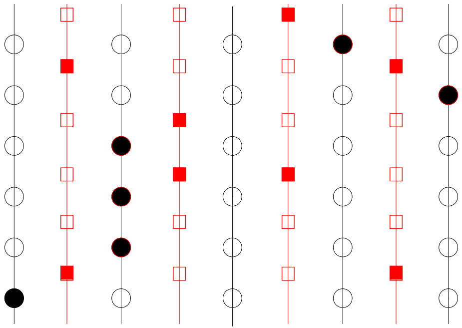
Diffusion



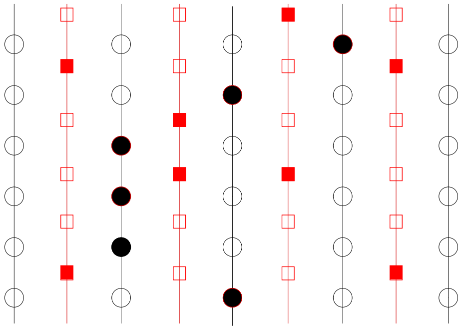
Diffusion



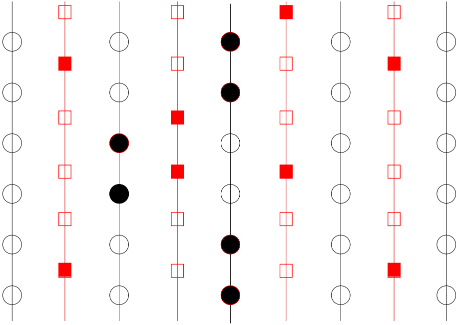
Diffusion



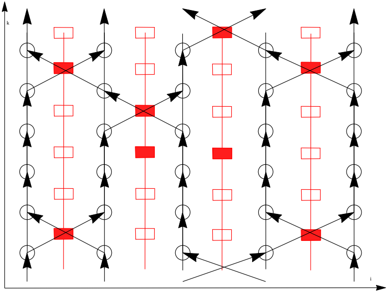
Diffusion



Diffusion



Coupling to particles reservoirs



Let $\sigma(\cdot;t-1)$, we define $\sigma(\cdot;t)$ for all $t\in\mathbb{N}^*$ by

$$\sigma(x;t)=\begin{cases}\sigma(F^{-1}(x);t-1) & \text{if} \quad x\notin B_-\cup B_+\\[2ex] \sigma_x^L(t-1) & \text{if} \quad x\in B_-\\[2ex] \sigma_x^R(t-1) & \text{if} \quad x\in B_+\end{cases}$$

$\{\sigma_x^L(t):x\in B_-,\, t\in\mathbb{N}\}$ and $\{\sigma_x^R(t):x\in B_+,\, t\in\mathbb{N}^*\}$ are independent Bernoulli variables of parameters respectively ρ_- and ρ_+.

Current of particles and Fick's law

d-dimensional version of the rings model.

$$\Lambda = \{1, \dots, N\}^d = \{i = (i_1, \dots, i_d), i_l \in \{1, \dots, N\},\ 1 \leq l \leq d\}.$$

The model consists of particles moving on :

$$\mathcal{C} = \prod_{i \in \Lambda} \mathcal{R}_i = \{(k, i) : k \in \{1, \dots, N\},\ i \in \Lambda\}.$$

We define the current of particles at time $t \in \mathbb{N}$ between hyperplanes $\mathcal{C}^l = \{x \in \mathcal{C} : i_d = l\}$ and $\mathcal{C}^{l+1}$, $l \in \{1, \dots, N-1\}$:

$$J(l, t) = \frac{1}{N^d} \sum_{(k,i) \in \mathcal{C}^l} c(k, i(i + e_d))(\sigma(k, i; t) - \sigma(k, i + e_d; t)),$$

where

$$c(k, ij) = \xi(k, ij) \prod_{\substack{l : d(i,l) = 1 \\ l \neq j}} (1 - \xi(k, il)) \prod_{\substack{l : d(j,l) = 1 \\ l \neq i}} (1 - \xi(k, jl))$$

and we set

$$\xi(k, ij) = 0.$$

whenever i or j do not belong to Λ.

Current of particles and Fick's law

Theorem

Let $d \geq 7$, $\rho_I, \rho_+, \rho_- \in (0,1)$ and ξ a family of Bernoulli random variables of parameter μ and $\{\sigma(x;0) : x \in \mathcal{C}\}$ be a set of independent Bernoulli random variables with $\mathbb{E}[\sigma(x;0)] = \rho_-$ if $x \in B_-$, $\mathbb{E}[\sigma(x;0)] = \rho_+$ if $x \in B_+$, and $\mathbb{E}[\sigma(x;0)] = \rho_I$ if $x \notin B_- \cup B_+$.

1. *For any $N \in \mathbb{N}^*$ and any $t \geq \bar{t} = N^{d+1}$, $J(l,t) = J(l,\bar{t}) := \overline{J}(l)$, the equality holds in law.*
2. *For any $\delta > 0$ and any $l \in 1, \ldots, N-1$,*

$$\lim_{N \to \infty} \mathbb{P}[\left| N\bar{J}(l) - \kappa(\mu)(\rho_- - \rho_+)\right| > \delta] = 0,$$

where $\kappa(\mu) = \mu(1-\mu)^{4d-2}$.

Proof : 3 steps-ingredients

- Relate the current to the number of crossings (for each configuration of scatterers)
- Relate the crossings to sample paths of lazy random walks for short times.
- Use the fact in high dimension random walks typically exit a finite box before making "loops" or intersecting each other.

Relation between current and number of crossings

$\mathcal{N}_\pm$ = the numbers of crossings from $B_\pm$ to $B_\mp = |S_\pm|$

$$S_\pm = \{x \in B_\pm : F^1(x) \notin B_\pm, \ldots, F^{s-1}(x) \notin B_\pm, F^s(x) \in B_\mp \text{ for some } s \in \mathbb{N}^*\}.$$

$\mathcal{N}_+ = \mathcal{N}_-$ because every orbit is closed. Set $\mathcal{N} = \mathcal{N}_+ = \mathcal{N}_-$.

Proposition

Let $\{\sigma(x;0) : x \in \mathcal{C}\}$ be a set of independent Bernoulli random variables with $\mathbb{E}[\sigma(x;0)] = \rho_\pm \in (0,1)$ if $x \in B_\pm$, and $\mathbb{E}[\sigma(x;0)] = \rho_I \in (0,1)$ if $x \notin B_- \cup B_+$. Then, for every $\delta > 0$, every ξ and every $t \geq N^{d+1}$,

$$\mathbb{P}\left[\left|J(l,t) - \frac{\mathcal{N}}{N^d}(\rho_- - \rho_+)\right| \geq \delta\right] \leq 2\exp(-\delta^2 N^d), l \in 1, \ldots, N-1.$$

- **For any fixed configuration of scatterers** ξ
- **The same holds for the mirrors model**

Proof of the theorem : two parts .

$$\mathbb{P}[\big|N\bar{J}(l) - \kappa(\mu)(\rho_- - \rho_+)\big| > \delta] \leq \mathbb{P}\left[\left|\bar{J}(l) - \frac{\mathcal{N}}{N^d}(\rho_- - \rho_+)\right| \geq \frac{\delta}{2N}\right] + \mathbb{P}\left[\left|\frac{N\mathcal{N}}{N^d}(\rho_- - \rho_+) - \kappa(\mu)(\rho_- - \rho_+)\right| \geq \frac{\delta}{2}\right]$$

$$\mathbb{E}[\frac{\mathcal{N}}{N^d}] = \frac{1}{N^d}\sum_{x \in B_-} \mathbb{E}[\mathbf{1}_{x \in S}] = \mathbb{P}[(1, \dots, 1) \in S]$$

$$\mathrm{Var}[\frac{\mathcal{N}}{N^d}] = \frac{1}{N^d}\sum_{x \in B_-} \mathbb{P}[(1, \dots, 1) \in S, x \in S] - \mathbb{P}[(1, \dots, 1) \in S]\mathbb{P}[x \in S]$$

To compute the probability, compare with a (lazy) random walk.

Compare to lazy random walks

$$x = (k,i) \to \begin{cases} v(x) = k \\ h(x) = i \end{cases} \qquad F^t(x) \to \begin{cases} v(F^t(x)) = V_t(x) \\ h(F^t(x)) = H_t(x) \end{cases}$$

$$t_L(x) = \inf\{t > 0 : \exists s < t,\ V_t(x) = V_s(x'),\ d(H_t(x), H_s(x)) \leq 3\}.$$

For any $x \in \mathcal{C}$,

$$\{H_s(x) : 0 \leq s \leq t_L(x)\}$$

has the same law than

$$\{W_s(h(x)) : 0 \leq s \leq \tau_L(h(x))\}$$

where $\{W_s(i) : s \in \mathbb{N}\}$ is the lazy symmetric random walk with parameter $\nu = \mu(1-\mu)^{4d-2}$ and

$$\hat{\mathbb{P}}[W_{t+1}(i) = j' | W_t(i) = j] = \begin{cases} \nu & \text{if} \quad d(j,j') = 1 & \\ 1 - 2d\nu & \text{if} \quad j = j' & j \notin b \\ 1 - (2d-1)\nu & \text{if} \quad j = j' & j \in b \\ 0 & \text{if} \quad d(j,j') > 1 & \end{cases} \tag{1}$$

$$\tau_L(i) = \inf\{t \in \mathbb{N}^*,\ \exists\, q \in \mathbb{N}^*, d(W_{t-qN}(i), W_t(i))| \leq 3\}.$$

For $d \geq 7$, one can show:

$$\mathbb{P}[(1,\dots,1) \in S] = \frac{1}{N}\mu(1-\mu)^{4d-2} + O(\frac{1}{N^{\frac{5}{2}}}).$$

because

$$\mathbb{P}[(1,\dots,1) \in S] = \mathbb{P}[(1,\dots,1) \in S, t_B < t_L] + \mathbb{P}[(1,\dots,1) \in S, t_B \geq t_L]$$

$$\mathbb{P}[(1,\dots,1) \in S] = \frac{1}{N}\mu(1-\mu)^{4d-2} + \mathcal{R}.$$

where $|\mathcal{R}| \leq 2\hat{\mathbb{P}}[\tau_L \leq \tau_B]$ and one can control the probability that a random walk makes a "loop" before exiting the system :

Proposition

If $d \geq 7$, for any $i \in \Lambda$ and any $N \in \mathbb{N}^*$

$$\hat{\mathbb{P}}[\tau_L(i) \quad \leq \quad \tau_B(i)] \leq C\frac{\mathbb{E}[\tau_B(i)]}{N^{d/2}}.$$

$$\tau_B(i) = \inf\{t \in \mathbb{N}^*, W_t(i) \in b\}.$$

For the variance

$$N^2\text{Var}[\frac{\mathcal{N}}{N^d}] = \frac{1}{N^{d-2}}\sum_{x\in B_-}\mathbb{P}[(1,\dots,1)\in S, x\in S] - \mathbb{P}[(1,\dots,1)\in S]\mathbb{P}[x\in S]$$

$$= \frac{1}{N^{d-2}}\sum_{x:d(x,\mathbf{1})\le N^{\frac{3}{4}}}(\dots) + \sum_{x:d(x,\mathbf{1})> N^{\frac{3}{4}}}(\dots)$$

Control the second term by :

Proposition

For i and i' in Λ such that $d(i,i') > N^{\frac{3}{4}}$ and $d \geq 7$,

$$\mathbb{P}[\tau_I(i,i') < \tau_B(i) \vee \tau_B(i')] \leq \frac{C}{N^{\frac{9}{4}}}.$$

where

$$\tau_I(i,i') = \tau_I(i \to i') \wedge \tau_I(i' \to i).$$

and

$$\tau_I(i \to i') = \inf\{t > 0 : \exists q \in \mathbb{N},\ d(W_t(i), W_{t-qN}(i')) \leq 2\},$$

Built on the classical result of Erdös and Taylor :

Proposition

Let $\{S_t(i) : t \in \mathbb{N}\}$ and $\{S_t(i') : t \in \mathbb{N}\}$ two independent symmetric random walks on $\mathbb{Z}^d$, with starting points $i, i' \in \Lambda$ such that $\rho = |i - i'| > 0$, then

$$\mathbb{P}[\{S_t(i) : t \in \mathbb{N}\} \cap \{S_t(i') : t \in \mathbb{N}\} \neq \emptyset] \leq \frac{C}{\rho^{d-4}}.$$

Conclusions

- Go to lower dimensions
- Consider the mirrors model
- Put correlations between scatterers.
- Large deviations
- ...