Macroscopic diffusion from a Hamilton-like dynamics

Raphaël Lefevere[1]

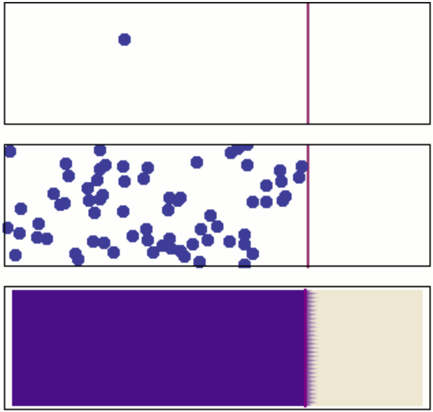
[1] Laboratoire de Probabilités et modèles aléatoires. Université Paris Diderot (Paris 7).

Louvain-la-Neuve, December 6th 2012.

From microscopic dynamics to macroscopic dynamics

Fick's Law :

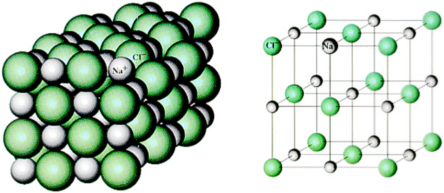
$$\partial_t \rho(x,t) = \partial_x (D(\rho)\partial_x \rho(x,t))$$



Rigorous result : diffusion in the Lorentz model.

Fourier Law in crystalline solids :

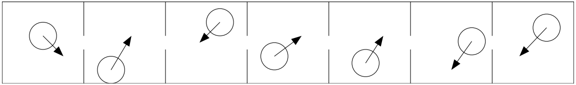
$$\partial_t T(x,t) = \partial_x(\kappa(T(x,t)\partial_x T(x,t))$$



Perturbation around a pathological case : harmonic interactions.

Fourier Law in aerogels :

$$\partial_t T(x,t) = \partial_x(\kappa(T(x,t)\partial_x T(x,t))$$

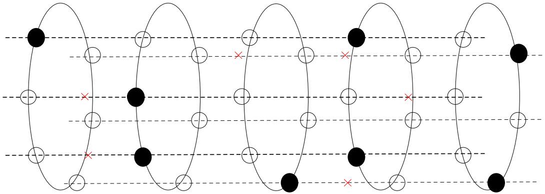


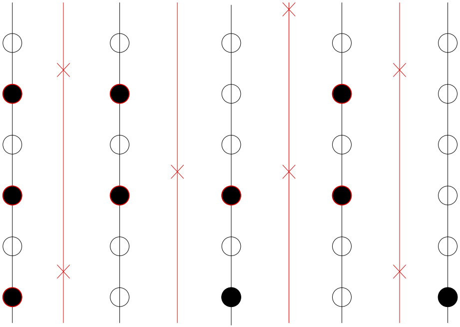
Possibility : take an individual cell to have the properties of a strongly chaotic billiard.

The set of models

- Fourier Law and Fick's law are everywhere : clearly they do not depend on delicate dynamical properties.
- The problem is maybe with the way we build microscopic models : typically we build them by taking a small model and then copy and paste it infinitely often as the number of components goes to infinity.
- It's hard to imagine and visualize the irregularity of the microscopic world.
- Build a set of toy models for Fick's law that have the characteristic properties of Hamiltonian dynamics and where one can play at will with the interactions between the components.
- Show that with "large probability'" the interactions will lead to macroscopic diffusion (in some limit)
- There are interactions for which no diffusion occur ! Perturbating around them is possible but probably very difficult.

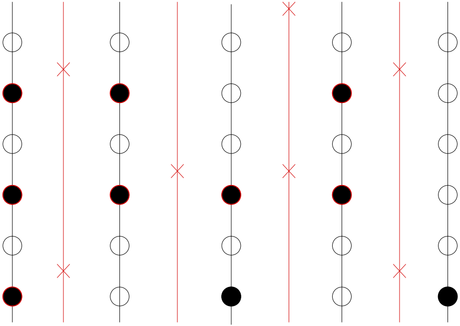
The set of models





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

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



A pair of neighbouring scatterers = no scatterer !
Dynamical system defined by the map $\tau : \mathcal{C}_N \to \mathcal{C}_N$:

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

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

Evolution of occupation variables

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

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

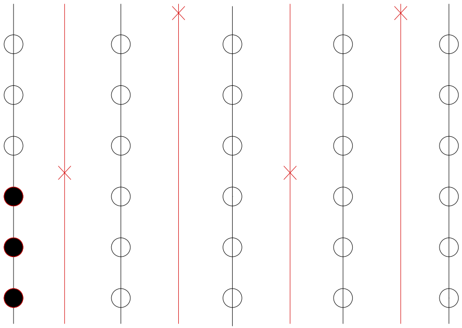
or recursion :

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

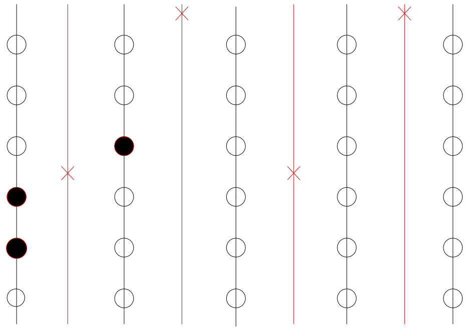
$\sigma(\cdot;t)$ is permutation of initial occupation variables $\sigma(\cdot;0)$.

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

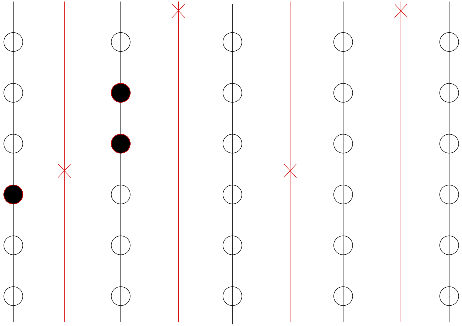
Interactions with no diffusion



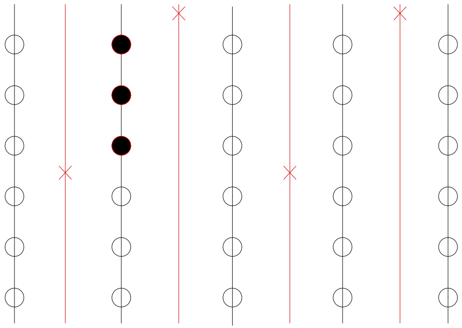
Interactions with no diffusion



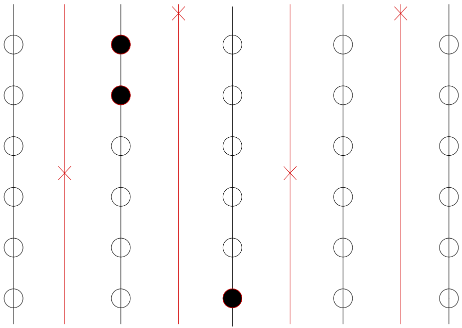
Interactions with no diffusion



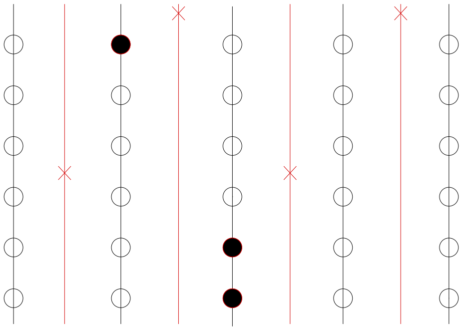
Interactions with no diffusion



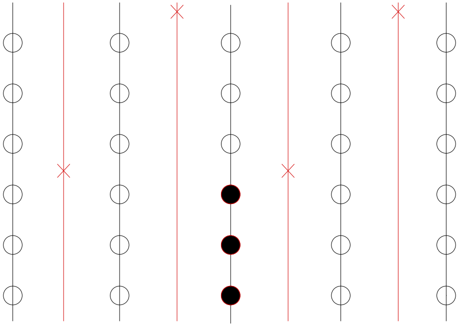
Interactions with no diffusion



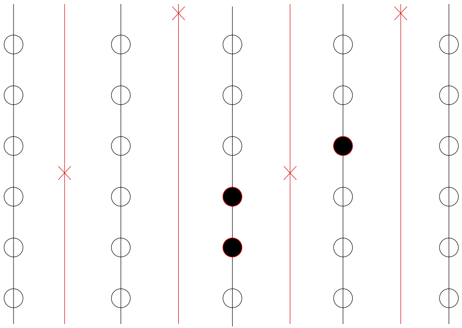
Interactions with no diffusion

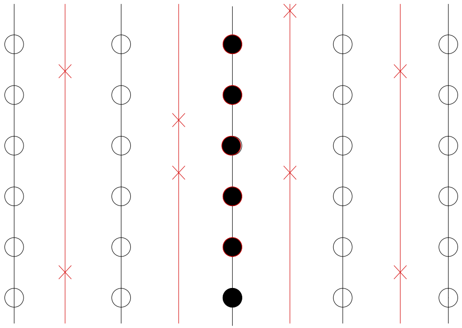


Interactions with no diffusion

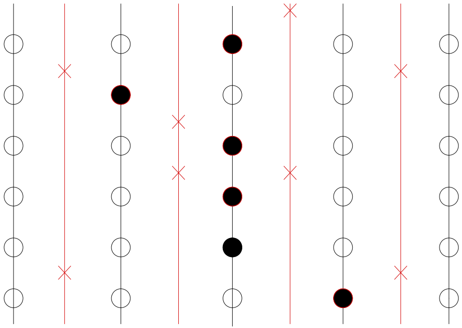


Interactions with no diffusion

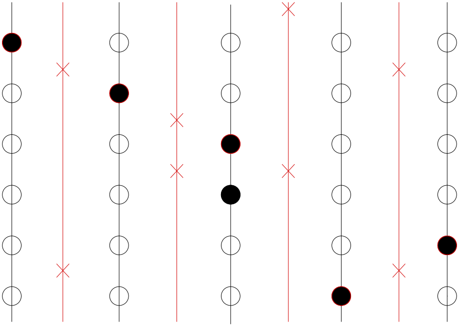




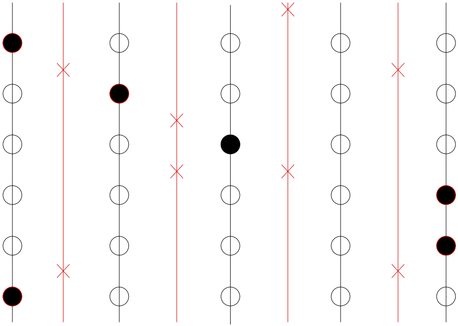
Diffusion



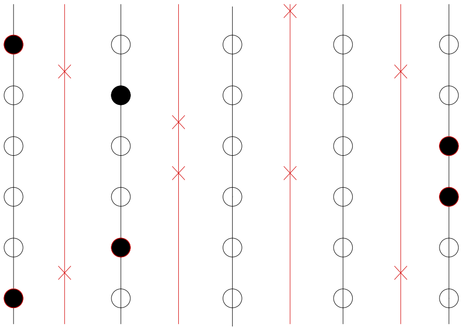
Diffusion



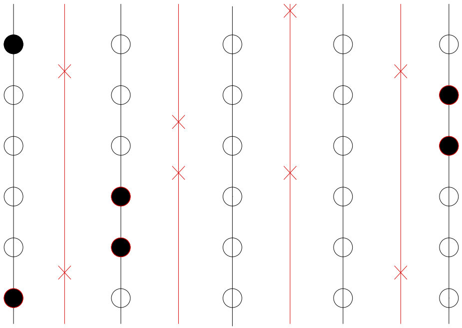
Diffusion



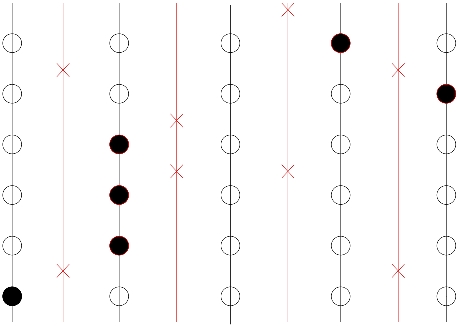
Diffusion



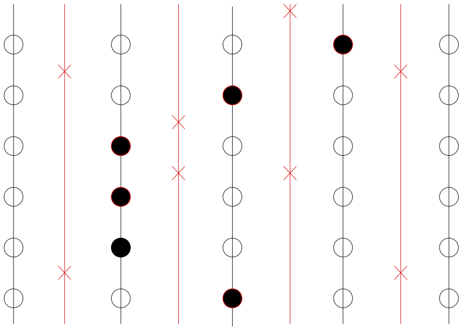
Diffusion



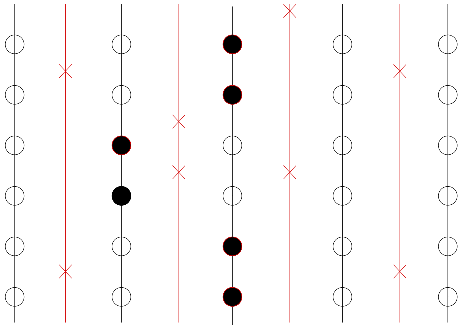
Diffusion



Diffusion



Diffusion



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 ?

No information on the “interactions” except its intensity or density , most natural choice is :

$$\xi(k,i) \sim \mathrm{Ber}(\mu).$$

Reference for the evolution of the macroscopic densities : solution of the equation :

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

Result: *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.*

Theorem

Let the $\{\sigma(k,i,0) : (k,i) \in \mathcal{C}_N\}$ *be a set of independent Bernoulli random variables and* $\{\hat{\rho}_i : 0 < \hat{\rho}_i < 1,\ i \in \Lambda_N\}$ *such that,* $\mathbb{E}(\sigma(k,i,0)) = \hat{\rho}_i$ *,* $\forall k \in \{1,\ldots,R\}$*. Let also* $\hat{\rho}(\cdot,t)$ *be the solution of the above system with initial condition* $\hat{\rho}(i,0) = \hat{\rho}_i$*,* $\forall \epsilon > 0$ *and* $\forall 0 < t < R^\alpha$ *with* $0 < \alpha < 1$*,*

$$\lim_{R\to\infty} \mathbb{P}\left[\bigcup_{i=-N}^{N} \{|\rho^R(i,t) - \hat{\rho}(i,t)| > \epsilon\}\right] = 0.$$

Proof

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

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.

Next, bound variance of the macroscopic density :

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

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

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

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*.

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

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 :

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

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',

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

Diffusion

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

Open questions

- Structure of the orbits
- Distribution of the periods : dependance on the order/disorder
- Same system connected to particles reservoirs
- Large deviations of the current
- Back to real Hamiltonian systems