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On the derivation of the laws of macroscopic diffusion

By

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Abstract

We report recent rigorous and numerical results obtained on the derivation of Fick's law for deterministic dynamics in random environment.

§ 1. Introduction

Ever since the works of the founding fathers of statistical mechanics, the derivation of the macroscopic laws of physics as the result of the motion of the microscopic components has been a major challenge which remains largely unsolved to this day. Fick's law is one of those central laws of macroscopic physics. It states that, after some transient time, the current of particles crossing an extended macroscopic system of length L decreases like the inverse power of L. A paradigmatic model in this context is provided by the Lorentz gas : it consists of tracer particles moving freely in a box and colliding with fixed obstacles. The only rigorous derivation of Fick's law was achieved by Bunimovich and Sinai in [1] for a finite horizon Lorentz gas when the scatterers have a specific shape that gives rise to a strongly chaotic dynamics. However, it is unlikely that the microscopic dynamics of a typical material possess the special properties of a strongly chaotic billiard. A more satisfactory result from a conceptual point of view would be to establish diffusion in a *random* Lorentz gas. In that case, obstacles of arbitrary shape

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are thrown at random in a box. The goal is to show that, after a diffusive rescaling of space and time is performed, macroscopic observables obey the laws of diffusion with very large probability with respect to the distribution of the obstacles. If one looks at Fick's law for the macroscopic current, this requires to control not only its average but also, at least, its variance. In contrast to the the Bunimovich-Sinai case, the randomness of the scatterers induce correlations between the trajectories and therefore also between occupation numbers (or local empirical densities) at different points in space. We report here the results of [3] and [2] on the derivation of Fick's law in the context of random Lorentz gas on a lattice also called the mirrors model. In [3], the model consists of a simplification of the original mirrors model. One direction of the lattice is special in the sense that the motion of every particle in that direction takes place at constant speed in that direction.

We recall now briefly the set-up of the original mirrors model. Particles travel on the edges of $\mathbb{Z}^2$ with unit speed. Mirrors are located at some vertices of the lattice and take two possible angular orientations : $\{\frac{\pi}{4}, \frac{3\pi}{4}\}$. When a particle hits a mirror, it gets deflected according to the laws of specular reflection, see Figure 2 for sample trajectories of particles. It is convenient to think that every particle starts at time zero with a given velocity at a vertex of the lattice $\mathcal{Q}$ that is obtained by taking the middle point of every edge of $\mathbb{Z}^2$. As all particles move with unit velocity, one can simply observe the evolution of the system at discrete times $t \in \mathbb{N}$. At those times, the particles will be always located at one of the vertices of the new lattice $\mathcal{Q}$ with a well-defined velocity. In general, the orientation of the mirrors is picked randomly. It is obvious that the motion of a single particle can not be described as a Markov process. When a particle hits a mirror for the second time, no matter how far back in the past the first visit occurred, its reflection is strongly affected by the way its was reflected at the first visit. For instance in Figure 2, the two orientations of the mirrors are picked at random, and in that case, at the second visit the reflection is always deterministic.

We come now to a more general definition of the dynamics in d dimensions. We denote by $\mathbf{z} = (z_1, \ldots, z_d)$ a generic element of $\mathbb{Z}^d$. As for $\mathbb{Z}^2$, we consider the set of midpoints of edges of an hypercube of $\mathbb{Z}^d$ of side N and with periodic conditions in all but the first direction. We call this set $\mathcal{Q}$. It may be described as follows : $\mathcal{Q} = \bigcup_{i=1}^d L_i$ where $L_i = \left\{\mathbf{z} + \frac{1}{2}\mathbf{e}_i : \ 0 \le z_1 \le N-1, \ (z_2, \ldots, z_d) \in (\mathbb{Z}/N\mathbb{Z})^{d-1}\right\}$. Let $(\mathbf{e}_1, \ldots, \mathbf{e}_d)$ the canonical basis of $\mathbb{R}^d$, the space of possible velocities is $\mathcal{P} = \{\pm\frac{\mathbf{e}_1}{2}, \ldots, \pm\frac{\mathbf{e}_d}{2}\}$ and the phase space of the dynamics is

$$\mathcal{M} = \{(\mathbf{q}, \mathbf{p}) : \mathbf{q} \in \mathcal{Q}, \mathbf{p} \in \mathcal{P} \text{ s. t. if } \mathbf{q} \in L_i \text{ then } \mathbf{p} = \pm\frac{\mathbf{e}_i}{2}\}.$$

We denote a generic point of $\mathcal{M}$ by $(\mathbf{q}, \mathbf{p})$. The set of points in $\mathcal{M}$ whose spatial coordinate belongs to the boundaries of the system is $B = B_- \cup B_+$, with

$$B_- = \{x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M} : \mathbf{q} = (q_1, \dots, q_d) \in L_1, q_1 = \frac{1}{2}\}$$
$$B_+ = \{x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M} : \mathbf{q} = (q_1, \dots, q_d) \in L_1, q_1 = N - \frac{1}{2}\}.$$

See Figure 1.

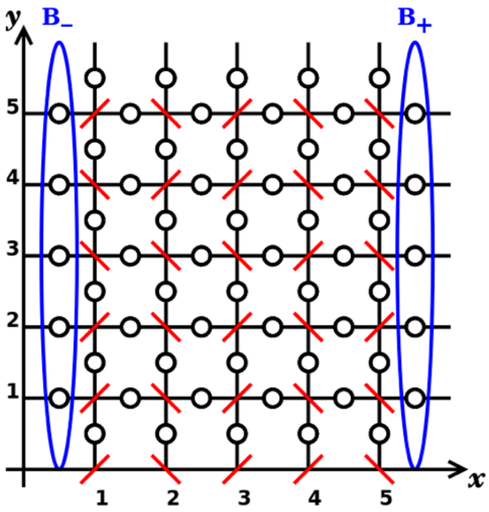

Figure 1. The spatial component of the phase space $\mathcal{M}$ and of the sets B_- and B_+ in $2D$.

For each $\mathbf{z} \in \mathbb{Z}^d$, we define the action of a "mirror" on the velocity of an incoming particle by $\pi(\mathbf{z}; \cdot)$ which is a bijection of $\mathcal{P}$ into itself. It satisfies the following conditions :

$$\begin{cases} \pi(\mathbf{z}; -\pi(\mathbf{z}; \mathbf{p})) = -\mathbf{p}, \quad \forall \mathbf{z} \in \mathbb{Z}^d, \forall \mathbf{p} \in \mathcal{P} \\ \pi(0, z_2, \dots, z_d; -\frac{\mathbf{e}_1}{2}) = \frac{\mathbf{e}_1}{2} \\ \pi(N, z_2, \dots, z_d; \frac{\mathbf{e}_1}{2}) = -\frac{\mathbf{e}_1}{2}, \; (z_2, \dots, z_d) \in (\mathbb{Z}/N\mathbb{Z})^{d-1} \end{cases} \tag{1.1}$$

The dynamics is defined on $\mathcal{M}$ in the following way. For any $(\mathbf{q}, \mathbf{p}) \in \mathcal{M}$:

$$F(\mathbf{q}, \mathbf{p}) = (\mathbf{q} + \mathbf{p} + \pi(\mathbf{q} + \mathbf{p}; \mathbf{p}), \pi(\mathbf{q} + \mathbf{p}; \mathbf{p}))\,.$$

The map F is a bijection on $\mathcal{M}$.

As we are interested in the transport of particles, we define occupation variables $\sigma(\mathbf{q}, \mathbf{p}; t) \in \{0, 1\}$ that record the absence or presence of a particle at position $\mathbf{q}$ with velocity $\mathbf{p}$ at time $t \in \mathbb{N}$. When connecting the system to external particles reservoirs, we obtain the following evolution rule : given $\sigma(\cdot; t-1)$, we define $\sigma(\cdot; t)$ for all $t \in \mathbb{N}^*$

by

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

The families of random variables $\{\sigma_x^-(t) : x \in B_-,\, t \in \mathbb{N}\}$ and $\{\sigma_x^+(t) : x \in B_+,\, t \in \mathbb{N}\}$ consist of independent Bernoulli variables with respective parameters ρ_- and ρ_+. If one chooses $\{\sigma(x;0) : x \in \mathcal{M}\}$ to be a collection of independent random variables, then it is easy to see by induction that at any $t \geq 0$, $\{\sigma(x;t) : x \in \mathcal{M}\}$ is a collection of i.i.d Bernoulli random variables. To simplify a bit the discussion, we choose an homogeneous initial distribution, i.e. all Bernoulli random variables have a common parameter ρ_I. We define the average current of particles that crosses the hyperplane $\mathcal{Q}^l = \{\mathbf{q} \in \mathcal{Q} : q_1 = l + \frac{1}{2}\}$, $l \in \{1, \dots, N-2\}$ during a diffusive time interval N^2 :

$$J(l,t) = \frac{1}{N^{d+1}} \sum_{s=t+1}^{t+N^2} \sum_{x \in \mathcal{M}} \sigma(x;s)\Delta(x,l) \tag{1.2}$$

where $\Delta(x,l) = 2(\mathbf{p} \cdot \mathbf{e}_1)\mathbf{1}_{\mathbf{q} \in \mathcal{Q}^l}$,with $x = (\mathbf{q}, \mathbf{p})$. Thus $\Delta(x,l)$ takes the value $+1$ (resp. -1) if x crosses the slice $\mathcal{Q}^l$ from left to right (resp. from right to left). We denote by $\mathcal{N}_\pm$ the numbers of crossings from $B_\pm$ to $B_\mp$ induced by F, i.e. $\mathcal{N}_\pm = |S_\pm|$ where $S_\pm$ is given by

$$S_\pm = \{x \in B_\pm : \exists s > 0, \forall 0 < j < s,\ F^j(x) \notin B_\pm, F^s(x) \in B_\mp\}.$$

One notes that $\mathcal{N}_+ = \mathcal{N}_-$. Indeed, since every orbit is closed, it must contain as many left-to-right than right-to-left crossings. Thus, we set $\mathcal{N} = \mathcal{N}_+ = \mathcal{N}_-$. A completely analogous definition for the current can be given for the current of particles for the rings model [3]. In both the mirrors model and the rings model, it is possible to obtain the

Theorem 1.1. *For any $t \geq |\mathcal{M}|$, $\mathbb{E}[J(l,t)] = \frac{\mathcal{N}}{N^{d-1}}(\rho_- - \rho_+)$. Moreover, for every $\delta > 0$, any $t \geq |\mathcal{M}|$ and $l \in \{1, \dots, N-2\}$,*

$$\mathbb{P}\left[\left|J(l,t) - \frac{\mathcal{N}}{N^{d-1}}(\rho_- - \rho_+)\right| \geq \delta\right] \leq 2\exp(-\delta^2 N^{d+1}). \tag{1.3}$$

We take now random configurations of reflectors $\{\pi(\mathbf{z};\cdot) : \mathbf{z} \in \mathbb{Z}^d\}$. The law of the reflectors is denoted by $\mathbb{Q}$. The map F becomes now a random map.

Definition 1.2. The model satisfies *Fick's law* if and only if there exists some $\kappa > 0$ (the conductivity) such that $\forall \delta > 0$,

$$\lim_{N\to\infty} \lim_{t\to\infty} \mathbb{P} \times \mathbb{Q}[|NJ(l,t) - \kappa(\rho_- - \rho_+)| > \delta] = 0. \tag{1.4}$$

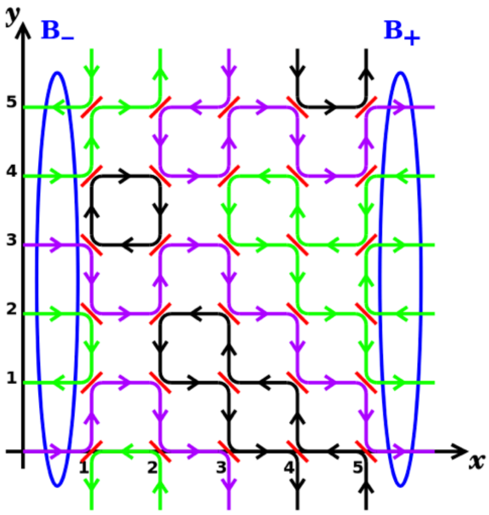

Figure 2. $N = 6$. Crossing orbits are coloured in purple, internal loops in black and non-crossing orbits are coloured in green. The travel direction given by the arrows is arbitrary. Each edge of the crossing orbits will be used twice in a given orbit : once in each direction. For this configuration of mirrors $\mathcal{N} = 2$.

It is easy to infer from (1.3) that the following theorem holds.

Theorem 1.3. Sufficient and Necessary Condition for Fick's law : *(1.4) holds if and only if there exists $\kappa > 0$ such that for any $\delta > 0$,*

$$\lim_{N\to\infty} \mathbb{Q}\left[\left|\frac{\mathcal{N}}{N^{d-2}} - \kappa\right| > \delta\right] = 0. \tag{1.5}$$

To go further, it is important to note that , using the notations $O = ((\frac{1}{2}, 0, \ldots, 0), \frac{\mathbf{e}_1}{2})$ and $S = S_-$:

$$\mathbb{E}\left[\frac{\mathcal{N}}{N^{d-2}}\right] = N\mathbb{Q}[O \in S] \tag{1.6}$$

and

$$\mathrm{Var}\left[\frac{\mathcal{N}}{N^{d-2}}\right] = \frac{1}{N^{2d-4}} \sum_{x,y\in B_-} \delta(x,y) = \frac{1}{N^{d-3}} \sum_{x\in B_-} \delta(O,x) \tag{1.7}$$

with

$$\delta(x,y) = \mathbb{Q}[x \in S, y \in S] - \mathbb{Q}[x \in S]\mathbb{Q}[y \in S]. \tag{1.8}$$

Next observe that if the law of an orbit with respect to $\mathbb{Q}$ was similar to the law of a simple random walk, then there would be a $\kappa > 0$ such that $\lim_{N\to\infty} N\mathbb{Q}[0 \in S] = \kappa$, this follows from the gambler's ruin argument. Similarly, if the orbits were independent objects, then the RHS of (1.7) would go to zero because the only non-zero term would be the one with $x = O$ and $\mathbb{Q}[O \in S] \sim \kappa/N$.

In [3], the equality (1.5) is proven for the rings model in $d \geq 7$. This is done by comparing the crossing probability $\mathbb{Q}[O \in S]$ to the crossing probability of a lazy random walk. The correction due to the memory effect in the real orbits give rise to a correction that decays in the size of the system faster than $1/N$. Correlations are treated in the same way.

In the mirrors model, we have tested the probability $\mathbb{Q}[O \in S]$ numerically [2]. The log-log plot of this probability versus the size of the system N is given in Figure 3. In order to show that the variance (1.7) goes to zero, we have also studied the

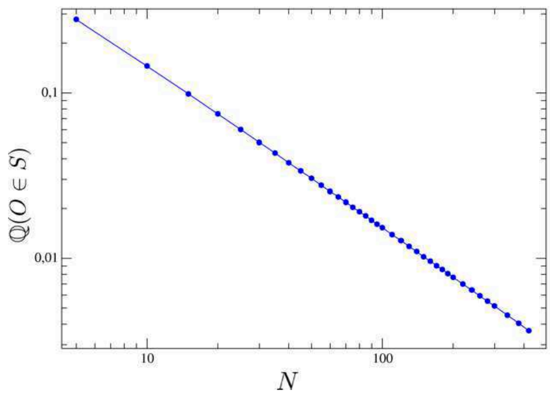

Figure 3. $\mathbb{Q}(O \in S)$ for N from 5 to 420. The 95% confidence interval is about half the size of a dot.

correlation functions $\delta(O,x)$ in $d = 3$. For all but a few points, the correlations $\delta(O,x)$ for $x \neq O$ are not only small but negative within confidence intervals, see Figure 4. The only exceptions are points $((1/2,1,0),\frac{\mathbf{e}_1}{2})$, $((1/2,0,1),\frac{\mathbf{e}_1}{2})$, $((1/2,N-1,0),\frac{\mathbf{e}_1}{2})$ and $((1/2,0,N-1),\frac{\mathbf{e}_1}{2})$ which give clearly positive correlations. However, we checked that for $N = 70$, $\sum_{y=1}^{N-1} \delta(O,((1/2,y,0),\frac{\mathbf{e}_1}{2})) = -1.360 \times 10^{-04} \pm 1.47 \times 10^{-05}$, i.e. it is negative with a margin of more than 9σ. $\sum_{z=1}^{N-1} \delta(O,((1/2,0,z),\frac{\mathbf{e}_1}{2}))$ must be equal by symmetry. Increasing values of N do not modify this behaviour. In particular, the number of points with positive correlations do not increase. Since we know already that $\mathbb{Q}[O \in S] \sim \kappa/N$, as $N \to \infty$, we conclude with the same margin that $\sum_{x\in B_-} \delta(O,x) \leq \kappa/N \to 0$, as $N \to \infty$. We expect the same behaviour in $d > 3$.

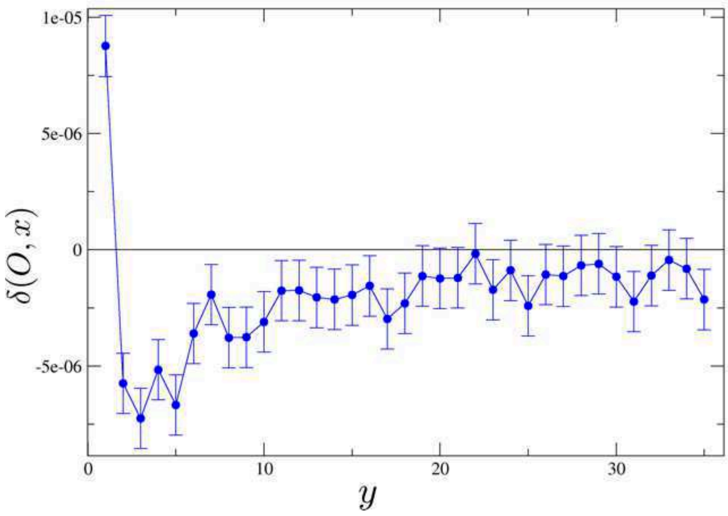

Figure 4. $\delta(O,x)$ for $x = ((1/2, y, 0), \frac{\mathbf{e}_1}{2})$. N=70. We draw the 95% confidence interval.

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