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Fick and Fokker–Planck diffusion law in inhomogeneous media

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Abstract We discuss particle diffusion in a spatially inhomogeneous medium. From the microscopic viewpoint we consider independent particles randomly evolving on a lattice. We show that the reversibility condition has a discrete geometric interpretation in terms of weights associated to un–oriented edges and vertices. We consider the hydrodynamic diffusive scaling that gives, as a macroscopic evolution equation, the Fokker–Planck equation corresponding to the evolution of the probability distribution of a reversible spatially inhomogeneous diffusion process. The geometric macroscopic counterpart of reversibility is encoded into a tensor metrics and a positive function. The Fick's law with inhomogeneous diffusion matrix is obtained in the case when the spatial inhomogeneity is associated exclusively with the edge weights. We discuss also some related properties of the systems like a non–homogeneous Einstein relation and the possibility of uphill diffusion.

Keywords Diffusion · Fick's law · Fokker–Planck diffusion law · hydrodynamic limit

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1 Introduction

The modelling of the diffusion of a physical quantity encoded by a *density field* $\rho(x,t)$ is usually constructed by assuming a continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot J \tag{1}$$

expressed in terms of the flux vectorial field $J(x,t)$ and a relation between the flux and the density field. The most popular choice is the *Fick's law* (see [16] for a very introductory discussion)

$$J = -D\nabla\rho \ , \tag{2}$$

where the positive function D is called *diffusion coefficient*. In general $D = D(\rho, x)$. When there is a dependence on ρ we obtain a nonlinear equation. For spatially homogeneous systems D does not depend on x.

Let us for simplicity consider the cases of a diffusion coefficient that does not depend on ρ. In many experimental situations [1,3,5–8,13,19,21,22,24,25] one should consider a not constant diffusion coefficient $D(x)$. In this cases it is not clear if Fick's law is the correct equation expressing the connection between the density and the flux fields. A different choice is the *Fokker–Planck diffusion law* (see the books [15,17] for an introduction to the Fokker–Planck equation)

$$J = -\nabla(D\rho) \tag{3}$$

which adds to the standard Fick's law a drift with velocity $-\nabla D$, see Section 4.2.

In correspondence of these two different assumptions one finds two possible equations for the diffusion problem

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D\nabla\rho) \tag{4}$$

and

$$\frac{\partial \rho}{\partial t} = \Delta(D\rho) \tag{5}$$

which will be respectively called the *Fick* and the *Fokker–Planck diffusion equation*; note that they reduce to the same equation if D is constant.

These two equations can be studied in $\Lambda \times [0,T]$ with $\Lambda \subset \mathbb{R}^d$ and $T > 0$ with $D \in C^2(\Lambda)$ and with initial condition $\rho(x,0) = \rho_0(x) \in C^2(\Lambda)$. Possible boundary conditions are Dirichlet or Neumann conditions on $\partial\Lambda$. In case Λ is a parallelepiped, it is possible to consider periodic boundary conditions.

In the applied science literature there are many situations in which the two different points of view are assumed. We just mention the paper [27] where

the Fick's law is used to study the transport of nutrients in cartilaginous tissues and the paper [22] where it is discussed an experiment in which a not uniform stationary density profile is produced starting from a uniform distribution of particles flowing inside a medium with not constant diffusion coefficient obtained by adding gelatine to water. This experimental observation is obviously in contrast with the Fick's law prediction.

The question whether diffusion in inhomogenous media should follow either Fick or Fokker–Planck equations has long been debated in the literature. For instance, Van Kampen in his classic textbook [17, Chapt.XI, Sec.3] considers a one–dimensional model on the real line in which a particle is "trapped" in a certain location for some time until it hops either leftwards or rightwards. Imposing the condition of detailed balance leads to the result that, in the appropriate scaling limit, one obtains Fick or Fokker–Planck law depending on the choice of the parameters.

The fact is that, as clearly explained in [25, 26], the question "what is the right generalization of the Fick's law to inhomogeneous systems" is too naive. A more detailed knowledge of the microscopic system is necessary to model correctly the macroscopic behavior. In [25] the authors, in particular, discuss a convincing and simple example based on two systems in which a closed box contains a very dilute gas moving through a dense mesh of iron wool. Model one: the iron wool density is uniform and the box experiences a fixed temperature gradient so that the typical particle speed varies continuously throughout the box. Model two: the temperature is uniform, but the iron wool density varies continuously in the box. The systems are designed so that the effective diffusion coefficient, which can be defined as the ratio between the square of the mean free path and the mean free time, is the same function of the space coordinates in the two systems. The authors remark that, since the temperature is uniform in box two and not uniform in box one they expect a stationary uniform particle density distribution in box two and not uniform in box one; indeed, they also deduce Fokker–Planck behavior for the first model and Fick for the second.

Our work is very much in the spirit of [25, 26], indeed, we assume the microscopic point of view and prove that two different models behave in the hydrodynamic limit [14,18] respectively according to the Fick and the Fokker–Planck diffusion law. In our modelling particles move in a discrete space and jump from one site to another following an edge. We find the Fick's behavior if the inhomogeneity is associated with edges and the Fokker–Planck one if inhomogeneity is associated with sites.

Our modelling provides a deep physical interpretation of the phenomenon, indeed, it suggests that the Fokker–Planck's law is associated with locally isotropic inhomogeneities, whereas inhomogeneity accompanied to anisotropy results into Fick's behavior. More precisely, suppose that in a small interval of time the number of particles leaving a site of the system is equally distributed among the edges intersecting that site, then the macroscopic behavior is Fokker–Planck. On the contrary, suppose that the number of particles leaving a site are not equally distributed among the edges intersecting that

site, but assume also that if two sites connected by an edge are occupied by the same number of particles then the number of particles moving along the bond in the two directions is equal. In such a case the macroscopic behavior is Fick. The second assumption assures that there is no preferred direction along an edge, in particular it rules out the possibility to have external fields acting on the system.

We note, finally, that our results are coherent with the simple example discussed in [25]. Consider a small portion of volume in the box one, the number of particles exiting the volume depends on its location due to velocity gradient. But, since the wool mesh is uniformly distributed, particles move with the same speed in all directions, so that the system is locally isotropic and this, accordingly to our results, implies the Fokker–Planck behavior. On the other hand, in box two the non–uniformity of the iron wool distribution breaks the local isotropy and this is why the Fick's behavior is found.

As we mentioned above the main goal of the paper is the derivation of the Fick and Fokker–Planck diffusion laws starting from a microscopic model in which the spatial inhomogeneity is differently implemented. The paper contains also a final section in which we discuss some relevant phenomena connected with inhomogeneous diffusion. In particular, we note that coupling a Fick channel with a Fokker–Planck one with suitable boundary conditions gives rise to the phenomenon of uphill currents, in the sense that the current will flow in the standard downhill direction in the Fick channel, namely, from the higher density end to the lower density one, whereas it will flow uphill in the Fokker–Planck channel. Moreover, in the same section we discuss the validity of an inhomogeneous Einstein relation.

The paper is organized as follows. In Section 2 we introduce the microscopic model and discuss some properties connected to invariant measures. In Section 3 we discuss the scaling limit of our class of inhomogeneous models. Finally, in Section 4 we report some additional remarks: heuristics and numerical simulations, a discussion on the situation with different lattice structure, the relation with the class of reversible continuous diffusions, Einstein relation, uphill current.

2 Models

We discuss here the microscopic structure of our inhomogeneous media.

2.1 Preliminaries

At microscopic level we have a graph with vertices V, and directed edges E. The corresponding set of unordered edges is denoted by F. A generic directed edge is denoted by $(x, y) \in E$ while an undirected one by $\{x, y\} \in F$. We consider always finite graphs such that if $\{x, y\} \in F$ then both (x, y) and (y, x) belong to E.

Two vertices $x, y \in V$ are said to be *neighbors* if and only if $\{x, y\} \in F$. We assume that the graph is *connected*, namely, for any pair of vertices $x, y \in V$ there exists a sequence of unordered edges $e_1, \dots, e_n \in F$ such that $x \in e_1$, $y \in e_n$, and $e_m \cap e_{m+1} \neq \emptyset$ for $m = 1, \dots, n-1$. For any $x \in V$ we let $C(x) \subset V$ be the set of vertices that are neighbors of x. The directed graph (V, E) is called strongly connected if for any pair of vertices $x, y \in V$ there exists a directed path going from x to y. We assume that our graphs are always strongly connected.

2.2 Random walks and particle systems

We consider one particle performing a Random Walk on the graph (V, E) with rates $r(x, y) > 0$ when $(x, y) \in E$. We say that the random walk is *reversible* if and only if there exists a probability measure $\mu(x)$ on V such that the *detailed balance condition*

$$\mu(x) r(x, y) = \mu(y) r(y, x)\,, \qquad \{x, y\} \in F \tag{6}$$

is satisfied. This condition can be satisfied only if $\{x, y\} \in F$ implies that both (x, y) and (y, x) belong to E. We stress again that this will be always true. If the condition (6) is satisfied then μ is invariant for the dynamics. This means that if the walker is distributed initially like μ its distribution does not change with time.

The *inhomogeneous random walk* (IRW) is the Markov jump process on the graph with transition rate from x to y given by

$$r(x, y) := \alpha(x) Q(\{x, y\})\,. \tag{7}$$

where $\alpha : V \to \mathbb{R}_+$ and $Q : F \to \mathbb{R}_+$ are arbitrary functions. We stress that Q is a function on un-ordered edges so that $Q(\{x, y\}) = Q(\{y, x\})$. To avoid irreducibility problems we assume that such functions are strictly positive. Sometimes we shall consider two particular cases in which the inhomogeneity is associated exclusively either with sites or bonds. The *site inhomogeneous random walk* (SIRW) is the IRW with $Q(e) = 1$ for any $e \in F$ and the *edge inhomogeneous random walk* (EIRW) is the IRW with $\alpha(x) = 1$ for any $x \in V$.

We can pass from the case of one single particle to that of M independent and indistinguishable particles letting $\eta(x)$ be the number of particles at site $x \in V$ and considering $\eta(x) r(x, y)$ as the rate at which one particle jumps from site x to site $y \in C(x)$. More formally, a configuration of particles is an element of the set $\Omega = \cup_{M=1}^{+\infty} \Omega_M$ with $\Omega_M := \{\eta \in \mathbb{N}^V, \sum_{x \in V} \eta(x) = M\}$. The value $\eta(x)$ is the number of particles at $x \in V$ and it is usually called the occupation variable at x. For $x, y \in V$ and $\eta \in \Omega$ such that $\eta(x) \geq 1$, we denote by $\eta^{x,y}$ the configuration obtained by η letting one particle jump from x to y. This means that, $\eta^{x,y}(x) = \eta(x) - 1$ and $\eta^{x,y}(y) = \eta(y) + 1$ while all

the remaining occupation variables remain the same. The stochastic evolution is encoded by the generator

$$\mathcal{L}f(\eta) = \sum_{(x,y)\in E} c_{x,y}(\eta)\left[f(\eta^{x,y}) - f(\eta)\right] , \tag{8}$$

with

$$c_{x,y}(\eta) = \eta(x)\alpha(x)Q(\{x,y\}) \tag{9}$$

and $f : \Omega \to \mathbb{R}$. The trajectories $(\eta_s)_{s\in[0,t]}$ of this Markov process belong to the space $D([0,t],\Omega)$. This is the space of the maps $\eta_\cdot : [0,t] \to \Omega$ that are right continuous and have limit from the left. We endow this space by the Skorokhod topology [4].

In the following we will denote by $\mathbb{P}_\nu$ the probability measure on $D([0,t],\Omega)$ determined by the Markovian stochastic evolution given by (8) when the particles are distributed at time 0 according to the measure ν. The corresponding expected value will be denoted by $\mathbb{E}_\nu$. The probability and the expected value with respect to a probability measure ν on Ω will be instead denoted respectively by E_ν and P_ν (or simply ν).

2.3 Invariant measures

Let us first discuss the case of one single particle. We claim that the class of all the reversible random walks on the graph G indeed coincides with the class of IRW.

Lemma 1 *A random walk on (V,E) is reversible if and only if the rates of transition are of the form (7). Moreover the invariant measure is $\mu(x) = 1/(\alpha(x)Z)$ where $Z = \sum_{y\in V}\alpha^{-1}(y)$ is a normalization constant.*

Proof Consider first a random walk with rates (7) and consider the probability measure $\mu(x) = 1/(\alpha(x)Z)$. Then the detailed balance condition (6) holds and the random walk is then reversible and the invariant measure is μ. Conversely consider a random walk for which (6) holds. Define then $Q(\{x,y\}) := \mu(x)r(x,y) = \mu(y)r(y,x)$ and $\alpha(x) = \mu^{-1}(x)$. Then with this choice of the weights formula (7) holds and we have therefore an IRW.

For the many particle system, the dynamic conserves the total number of particles and consequently in absence of particle sources there will be a family of invariant measures depending on the number of particles. On each subset Ω_M the dynamics is irreducible and there will be a corresponding unique invariant measure.

It will be more convenient to work with the grand canonical invariant measures that are obtained as special convex combinations of the canonical ones. The family of grand canonical invariant measures is parameterized by a

parameter related to the averaged density. Given a function $\lambda(\cdot) : V \to \mathbb{R}$ we define an associated inhomogeneous product Poisson measure

$$\mu^{\lambda(\cdot)}(\eta) = \prod_{x \in V} e^{-\lambda(x)} \frac{\lambda(x)^{\eta(x)}}{\eta(x)!} \,. \tag{10}$$

When $\lambda(\cdot) = \lambda$ is a constant function we call simply μ^{λ} the corresponding homogeneous product measure. The measure (10) satisfies the detailed balance condition provided $\lambda(x) = c\alpha^{-1}(x)$ for an arbitrary constant c. We obtain in this way a family of grand canonical invariant measures depending on the free parameter c. We note that the average number of particles at site $x \in V$ under the measure $\mu^{\lambda(\cdot)}$ is $E_{\mu^{\lambda(\cdot)}}[\eta(x)] = \lambda(x)$. We have therefore for the grand canonical stationary measures $E_{\mu^{c\alpha^{-1}(\cdot)}}(\eta(x)) = c\alpha^{-1}(x)$.

Conversely, the canonical measures are obtained by the grand canonical ones conditioning on the total number of particles. More precisely we have

$$\nu^{M}(\eta) = \mu^{c\alpha^{-1}(\cdot)} \left(\eta \Big| \sum_{x \in V} \eta(x) = M \right) ,$$

and the conditioning is independent from the parameter c of the grand canonical measure.

3 Scaling limits

3.1 Microscopic and macroscopic observables

In order to perform the scaling limits we need to introduce a general framework and some observables. We will give a microscopic and a macroscopic description of the system. The macroscopic domain Λ is in general a bounded domain of $\mathbb{R}^d$, but to avoid dealing with boundary conditions we consider the d dimensional torus $[0,1]^d$ with periodic boundary conditions. The discretization of the macroscopic domain is $\Lambda_N := (\mathbb{Z}/N)^d \cap \Lambda$ that will be the set of vertices denoted before as V, with edges between nearest neighbors sites. We call respectively E_N and F_N the oriented and the un–oriented edges of the graph. We denote by $\mathcal{L}_N$ the generator of the process (8) when the underlying graph is (Λ_N, E_N). In general, a lower index N is used to denote the fact that the graph that we are considering is the lattice Λ_N with the corresponding edges.

A discrete vector field ϕ is a map $\phi : E_N \to \mathbb{R}$ such that $\phi(x,y) = -\phi(y,x)$. A vector field ϕ is of gradient type if there exists a function $f : V \to \mathbb{R}$ such that $\phi(x,y) = f(y) - f(x)$. In this case we write $\phi = \nabla f$.

Given a smooth function $f : \Lambda \to \mathbb{R}$, its discretized version f_N on the lattice Λ_N is defined by $f_N(x) = f(x)$, $x \in \Lambda_N$ (with abuse of notation we

drop sometimes the index N). Given a smooth vector field $\psi : \Lambda \to \mathbb{R}^d$ a natural discretization is obtained for example considering the line integral

$$\psi_N(x,y) := \int_{(x,y)} \psi(z) \cdot dl\,, \quad (x,y) \in E_N\,. \tag{11}$$

We have that ψ_N is a discrete vector field.

Consider a collection of smooth weight functions $Q = (Q_1, \dots, Q_d) : \Lambda \to (\mathbb{R}_+)^d$. We consider a corresponding discretized version as a weight function Q_N taking values on $\mathbb{R}_+$ and defined on the un-oriented edges by

$$Q_N(\{x,y\}) := Q_i\left(\frac{x+y}{2}\right)\,, \qquad \{x,y\} \in F_N\,, \tag{12}$$

where i in (12) has to be fixed in such a way that $y = x \pm e^i$ where e^i is the vector of modulus N^{-1} and directed as the i coordinate axis. Note that this discretization is very different with respect to (11) since in that case $\psi_N(x,y)$ is of order $1/N$ while in this case $Q_N(\{x,y\})$ is of order 1.

The general situation that we imagine is that the weights on the edges are the discretization Q_N of positive smooth weight functions while the weights on the vertices are the discretization α_N of a positive smooth function.

The empirical measure $\pi_N(\eta)$ is a positive measure on Λ, with finite total mass, i.e. an element of $\mathcal{M}^+(\Lambda)$, associated to a configuration of particles η and defined by

$$\pi_N(\eta) := \frac{1}{N^d} \sum_{x \in \Lambda_N} \eta(x)\delta_x \tag{13}$$

where δ_x is the delta measure. According to this definition, given a continuous function $f : \Lambda \to \mathbb{R}$ we have

$$\int_\Lambda f\, d\pi_N(\eta) = \frac{1}{N^d} \sum_{x \in \Lambda_N} \eta(x) f(x).$$

We endow $\mathcal{M}^+(\Lambda)$ with the weak topology. We say that a sequence of configurations η (for each N we have a configuration of particles on Λ_N, for simplicity of notation the dependence on N is understood) is associated to a density profile $\rho \in L^1(\Lambda)$ if $\pi_N(\eta) \to \rho(x)dx$ where $\to$ denotes the weak convergence on $\mathcal{M}^+(\Lambda)$. This means that for any continuous function f (recall that Λ is compact) we have

$$\lim_{N \to +\infty} \int_\Lambda f\, d\pi_N(\eta) = \int_\Lambda f(x)\rho(x)dx\,.$$

Likewise a sequence of probability measures μ_N on the configurations of particles $\mathbb{N}^{\Lambda_N}$ is said to be associated with a density profile ρ if for any continuous function f and for any $\epsilon > 0$ we have

$$\lim_{N \to +\infty} P_{\mu_N}\left(\left|\int_\Lambda f\, d\pi_N(\eta) - \int_\Lambda f(x)\rho(x)dx\right| > \epsilon\right) = 0\,. \tag{14}$$

3.2 Large deviations and free energy

We discuss firstly the scaling limit for the empirical measure when the particles are distributed according to a grand canonical invariant measure.

We show the result for a generic continuous function $\lambda(\cdot)$ recalling that the grand canonical invariant measure is obtained setting $\lambda(\cdot) = c\alpha^{-1}(\cdot)$ for a suitable c. Since the measure is of product type this is a classic problem and we show not only the scaling limit but also the corresponding large deviations asymptotics [18, 23]. In this case given a continuous function f, we obtain by a direct computation

$$V^*(f) := \lim_{N\to+\infty} \frac{1}{N^d} \log E_{\nu_N^{\lambda(\cdot)}} \left[e^{N^d \int_\Lambda f d\pi_N(\eta)} \right] = \int_\Lambda \lambda(x)(e^{f(x))} - 1)\, dx\,. \quad (15)$$

According to general results on large deviations [23] the corresponding large deviations rate functional, on $\mathcal{M}^+(\Lambda)$ endowed with the weak convergence, is given by

$$V(\rho) = \sup_{f\in C(\Lambda)} \left[\int_\Lambda f\, d\rho - V^*(f) \right]. \quad (16)$$

This gives a rate functional V that is $+\infty$ if the positive measure ρ is not absolutely continuous and when $\rho = \rho(x)\, dx$ we have

$$V(\rho) = \int_\Lambda \left[f(\rho(x)) - f(\lambda(x)) - f'(\lambda(x))\,(\rho(x) - \lambda(x)) \right] dx \quad (17)$$

where $f(\rho) = \rho \log \rho$ is the density of free energy for a system of independent particles. Here and hereafter with call with the same name an absolutely continuous measure and the corresponding density.

The form of the rate functional (17) has a structure similar to the one corresponding to a spatially homogeneous system. The only difference is that in (17) $\lambda(x)$ has to be substituted by a constant corresponding to the typical density. Recall instead that $\lambda(x) = c\alpha^{-1}(x)$ for the inhomogeneous grand canonical measure.

The functional (17) plays the role of a thermodynamic potential and its probabilistic interpretation is that roughly we have

$$P_{\mu_N^{\lambda(\cdot)}} \left(\pi_N(\eta) \sim \rho(x)dx \right) \simeq e^{-N^d V(\rho)}\,, \quad (18)$$

where $\sim$ means closeness in the weak topology and $\simeq$ means asymptotic logarithmic equivalence (see [23] for a precise statement). In particular, since $V(\rho) = 0$ if and only if $\rho(x) = \lambda(x)$, from (18) we can deduce the scaling limit of the empirical measure when the particles are distributed according to the invariant measure. We have indeed that $\pi_N(\eta) \to \bar\rho(x)dx = c\alpha^{-1}(x)dx$, weakly $\mu_N^{c\alpha^{-1}(\cdot)} a.e.$.

3.3 Dynamic scaling limit

We deduce in this section the diffusive scaling limit of many independent IRW's on the lattice Λ_N. This means that we consider a system of particles defined by the rates (9). This system has a diffusive behavior and this means that we have to multiply by N^2 the rates of jump that corresponds to accelerating by the same scale factor the time.

The proof of our result follows the general strategy outlined in [18] for gradient reversible models with the simplifying feature that we have independent particles. We give an outline of the proof underlying the modifications that we have to do in order to keep into account the spatial inhomogeneity of the models.

Given ν_N and μ_N two sequences of probability measures on the configuration of particles Ω and such that ν_N is absolutely continuous with respect to μ_N we introduce their relative entropy defined by

$$H\left(\nu_N|\mu_N\right) := E_{\nu_N}\left[\log\frac{\nu_N(\eta)}{\mu_N(\eta)}\right]. \tag{19}$$

If $c_{x,y}(\eta)$ is the rate at which one particle jumps from x to y in the configuration η we define the instantaneous current as

$$j_\eta(x,y) := c_{x,y}(\eta) - c_{y,x}(\eta)\,. \tag{20}$$

This is a discrete vector field for any fixed configuration η. Recalling (9) we have that the instantaneous current is given by

$$j_\eta(x,y) = Q(\{x,y\})\left[\alpha(x)\eta(x) - \alpha(y)\eta(y)\right]. \tag{21}$$

Recall also that to get a non–trivial scaling limit we will accelerate the process by a factor of N^2 so that the instantaneous current (21) will be multiplied by N^2.

We have the following.

Theorem 1 *Consider a collection of IRW's associated to the discretization of C^2 smooth and strictly positive weights α and Q. Consider ρ_0 an element of $L^1(\Lambda, dx)$. Let ν_N be a sequence of probability measures on the configuration of particles Ω associated to the profile ρ_0 in the sense of* (14) *and such that there exists a positive constant K and a constant λ such that*

$$H\left(\nu_N|\mu_N^\lambda\right) \le KN^d\,. \tag{22}$$

When the rates in (8) *are multiplied by N^2 we have that for any t, for any continuous function f and for any $\epsilon > 0$*

$$\lim_{N\to+\infty}\mathbb{P}_{\nu_N}\left(\left|\int_\Lambda f\,d\pi_N(\eta_t) - \int_\Lambda f(x)\rho(x,t)dx\right| > \epsilon\right) = 0\,, \tag{23}$$

where $\rho(x,t)$ is the unique weak solution of the equation

$$\begin{cases} \partial_t \rho = \nabla \cdot \Big(\mathbb{Q} \nabla \Big(\alpha \rho \Big) \Big) \\ \rho(x,0) = \rho_0(x) \end{cases} \tag{24}$$

and $\mathbb{Q}$ is the diagonal matrix having elements $\mathbb{Q}_{i,j}(x) := Q_i(x)\delta_{i,j}$.

Proof Preliminaries: Consider a smooth test function $f(s,x) : \mathbb{R}^+ \times \Lambda \to \mathbb{R}$ and the associated martingales (see for example [18] Appendix 1 Section 5)

$$\begin{aligned} M^f(t) := & \int_\Lambda f(t)\, d\pi_N(\eta_t) - \int_\Lambda f(0)\, d\pi_N(\eta_0) \\ & - N^{-d} \sum_{x \in \Lambda_N} \int_0^t ds \left(\partial_s f(s,x) \eta_s(x) + f(s,x) N^2 \mathcal{L}_N \eta_s(x) \right) . \end{aligned} \tag{25}$$

$$B^f(t) := \left(M^f(t) \right)^2 - \int_0^t \Gamma^f(s) ds \tag{26}$$

where

$$\begin{aligned} \Gamma^f(t) := & N^2 \mathcal{L}_N \left(\int_\Lambda f(t)\, d\pi_N(\eta_t) \right)^2 \\ & - 2N^2 \left(\int_\Lambda f(t)\, d\pi_N(\eta_t) \right) \mathcal{L}_N \left(\int_\Lambda f(t)\, d\pi_N(\eta_t) \right) . \end{aligned}$$

The second term (without the minus sign) on the right hand side of (26) is called the quadratic variation of the martingale M^f. A direct computation gives

$$\Gamma^f(t) = \frac{N^2}{2N^{2d}} \sum_{\{x,y\} \in F_N} Q(\{x,y\}) \big(f(t,x) - f(t,y) \big)^2 \left(\alpha(x)\eta_t(x) + \alpha(y)\eta_t(y) \right) . \tag{27}$$

Since f, α, Q are C^2, using (27), we have that

$$\Gamma^f(t) \le \frac{C}{N^{2d}} \sum_{x \in \Lambda_N} \eta_t(x) \tag{28}$$

for a suitable constant C. This is a key estimate in our computations that is similar to the estimate that holds in the homogeneous case. This fact allows us to extend the results in the homogeneous case to the non–homogeneous one.

With a discrete integration by parts the third term on the right hand side of (25) (without the minus sign) becomes

$$\int_0^t ds \int_\Lambda \partial_s f(s)\, d\pi_N(\eta_s) + \frac{N^2}{2N^d} \sum_{(x,y) \in E_N} \int_0^t \left(f(s,y) - f(s,x) \right) j_{\eta_s}(x,y)\, ds\,. \tag{29}$$

Using the expression (21) of the rates and performing another discrete integration by parts, the second term in (29) becomes

$$\frac{1}{N^d}\sum_{x\in\Lambda_N}\int_0^t \alpha(x)\eta_s(x)\left[N^2\sum_{y\in C(x)} Q(\{x,y\})\,(f(s,y)-f(s,x))\right]. \tag{30}$$

Inside squared parenthesis in the above formula we have a discrete operator acting on the test function f and not depending on configurations of particles. We need to understand which is the corresponding continuous differential operator. Since our rates are obtained by discretizing smooth functions we obtain with a Taylor expansion of Q that the term inside the squared parenthesis in (30) can be written, up to a term $O(1/N)$, as

$$\begin{aligned}\sum_{i=1}^d \Big[Q_i(x)N^2\left(-2f(s,x)+f\left(s,x+e^i\right)+f(s,x-e^i)\right)\\ +\frac{N}{2}\partial_{x_i}Q_i(x)(f(s,x+e^i)-f(s,x-e^i))\Big].\end{aligned} \tag{31}$$

Recall that e^i is the vector associated to the i Cartesian axis and having modulus $1/N$. The expression inside the squared parenthesis in (31) is then equal to

$$\nabla\cdot(\mathbb{Q}(x)\nabla f(s,x))$$

up to a infinitesimal term uniform over x. We obtain, therefore, that

$$N^{2-d}\sum_{x\in\Lambda_N}\int_0^t ds\, f(s,x)\mathcal{L}_N\eta_s(x)=\int_0^t ds\int_\Lambda \alpha\nabla\cdot(\mathbb{Q}\nabla f(s))\; d\pi_N(\eta_s)+\mathcal{R}_N(t)\,, \tag{32}$$

where the residual term $\mathcal{R}_N(t)$ can be bounded by

$$|\mathcal{R}_N(t)|\le\frac{Ct\int_\Lambda d\pi_N(\eta_0)}{N}$$

for a suitable constant C. We used the fact that the dynamics is conservative and we have $\int_\Lambda d\pi_N(\eta_s)=\int_\Lambda d\pi_N(\eta_0)$ for any s.

Since the initial configuration is associated to an integrable profile ρ_0, selecting as a test function in the definition (14) (with ρ replaced by ρ_0 and μ_N by ν_N) a function constantly equal to 1, we deduce

$$\mathbb{P}_{\nu_N}\left(\sup_{0\le s\le t}|\mathcal{R}_N(s)|>\epsilon\right)\le P_{\nu_N}\left(\int_\Lambda d\pi_N(\eta)>\frac{\epsilon N}{Ct}\right)\overset{N\to+\infty}{\to}0\,,\qquad\forall\epsilon>0\,. \tag{33}$$

Tightness: Let us call $\mathcal{P}_N:=\mathbb{P}_{\nu_N}\cdot\pi_N^{-1}\in\mathcal{M}^1\big(D([0,t];\mathcal{M}^+(\Lambda))\big)$ (endowed of the Skorokhod topology) the probability measure corresponding to the distribution of $(\pi_N(\eta_s))_{s\in[0,t]}\in D([0,t];\mathcal{M}^+(\Lambda))$. The first step consists in proving that the sequence of probability measures $\mathcal{P}_N$ is relatively compact. As it

is discussed in [18] chapters 4 and 5, we need to prove relative compactness of the marginals for any fixed time and in addition we need to have a control concerning oscillations in time.

Since the total mass is preserved by the dynamics to prove the relative compactness of any marginal it is enough to prove it for the initial condition. Since Λ is compact we need just to control the total mass. In particular we need to prove

$$\lim_{A\to+\infty}\limsup_{N\to+\infty} P_{\nu_N}\left(\int_\Lambda d\pi_N(\eta) > A\right) = 0\,. \tag{34}$$

This is obtained by the same argument used for (33).

To control oscillations we use the Aldous criterion (see [18] chapter 4 Proposition 1.6). Using arguments similar [18] chapter 4 Section 2 we deduce that a sufficient condition is

$$\lim_{\gamma\to 0}\limsup_{N\to+\infty}\frac{C\gamma}{N^d}E_{\nu_N}\left(\int_\Lambda d\pi_N(\eta)\right) = 0\,. \tag{35}$$

If we prove that the expected value in the above formula is bounded then the result follows. To this end it is not enough that ν_N is associated to an integrable profile. At this point it is relevant the entropy condition. Recall the basic entropy inequality (see for example [18] appendix 1 Section 8). Given two probability measures μ and ν and a function f we have

$$E_\nu(f) \le \beta^{-1}\left[\log E_\mu\left(e^{\beta f}\right) + H(\nu|\mu)\right]\,, \tag{36}$$

where β is an arbitrary parameter. We apply this inequality considering $\nu = \nu_N$, $\mu = \mu_N^\lambda$, $\beta = N^d$ and finally $f(\eta) = \int_\Lambda d\pi_N(\eta)$. We obtain

$$\begin{aligned} E_{\nu_N}\left(\int_\Lambda d\pi_N(\eta)\right) &\le \frac{1}{N^d}\left(\log E_{\mu_N^\lambda} e^{\sum_{x\in\Lambda_N}\eta(x)} + H(\nu_N|\mu_N^\lambda)\right) \\ &\le e^{\lambda(e-1)} + K_0, \end{aligned} \tag{37}$$

where we used the hypothesis on the relative entropy of the initial condition and the explicit form of the generating function of a Poisson distribution. The proof of tightness is concluded.

Absolute continuity: Using again the entropy inequality it is possible to show that the bound on the relative entropy for the initial distribution is still valid with respect to a slowly varying product of exponentials $\mu_N^{\lambda(\cdot)}$.

Considering $\lambda(\cdot) = c\alpha^{-1}(\cdot)$ we have that $\mu_N^{\lambda(\cdot)}$ is invariant for the dynamics and we have therefore (see [18] appendix 1 Section 9) that $H\left(\nu_N(t)|\mu_N^{\lambda(\cdot)}\right)$ is decreasing in time where $\nu_N(t)$ is the distribution of particles at time t. This means that for any $t \ge 0$ we have $H\left(\nu_N(t)|\mu_N^{\lambda(\cdot)}\right) \le N^d C$ for a suitable constant C. This is the basic fact on which it is based the argument in [18] Section 1. In particular Lemma 1.6 there, should be rewritten considering in this case I_0 coinciding with the large deviations rate functional V in (17).

We deduce that any possible limit point $\mathcal{P}^*$ of any subsequence in $\mathcal{P}_N$ is concentrated on elements of $D([0,t],\mathcal{M}^+)$ that are of the form $\rho(x,s)dx$ for any $s\in[0,t]$ and $\rho(x,s)\in L^1(\Lambda)$.

Characterization of limit points: Since the sequence of probability measures $\mathcal{P}_N$ is relatively compact we can extract a converging subsequence. For simplicity of notation we call again $\mathcal{P}_N$ this converging subsequence and $\mathcal{P}^*$ its limit point.

Let us consider the martingale (25). By the Chebysev and the Doob inequality we have

$$\mathbb{P}_{\nu_N}\left(\sup_{0\le s\le t}|M^f(s)|>\epsilon\right)\le\frac{4\mathbb{E}_{\nu_N}\left[\left(M^f(t)\right)^2\right]}{\epsilon^2}=\frac{4\int_0^t\mathbb{E}_{\nu_N}\left[\Gamma^f(s)\right]\,ds}{\epsilon^2}\,. \quad (38)$$

Recalling the bounds (28) and (37) we have that the right hand side of (38) is bounded by $\frac{4Ct}{\epsilon^2N^d}$ for a suitable constant C and this is converging to zero when $N\to+\infty$.

Let us call

$$\begin{aligned}\tilde{M}^f(t):=&\int_\Lambda f(t)d\pi_N(\eta_t)-\int_\Lambda f(0)d\pi_N(\eta_0)\\&-\int_0^t ds\int_\Lambda\left[\partial_s f(s)+\alpha\nabla\cdot(\mathbb{Q}\nabla f(s))\right]\,d\pi_N(\eta_s)\,.\end{aligned} \quad (39)$$

First we recall that by (32) we have $M^f(t)-\tilde{M}^f(t)=\mathcal{R}_N(t)$, that is uniformly negligible in probability according to (33). Second we observe that the map that associate to any $\pi(s)\in D([0,t],\mathcal{M}^+(\Lambda))$ the number

$$\sup_{0\le w\le t}\left|\int_\Lambda f(w)d\pi(w)-\int_\Lambda f(0)d\pi(0)-\int_0^w ds\int_\Lambda[\partial_s f(s)+\alpha\nabla\cdot(\mathbb{Q}\nabla f(s))]\,d\pi(s)\right|$$

is a continuous function in the Skorokhod topology of $D([0,t],\mathcal{M}^+(\Lambda))$.

Since by assumption we have that the subsequence $\mathcal{P}_N$ is weakly converging to $\mathcal{P}^*$, by Portmanteau Theorem we have for any $\epsilon>0$

$$\begin{aligned}\mathcal{P}^*\Big(\sup_{0\le w\le t}\Big|\int_\Lambda f(w)d\pi(w)-\int_\Lambda f(0)d\pi(0)-\int_0^w\Big[\partial_s f(s)\\+\int_\Lambda\alpha\nabla\cdot\Big(\mathbb{Q}\nabla f(s)\Big)\Big]\,d\pi(s)\Big|>\epsilon\Big)\\\le\liminf_{N\to+\infty}\mathbb{P}_{\nu_N}\Big(\sup_{0\le w\le t}\Big|M^f(w)-\mathcal{R}_N(w)\Big|>\epsilon\Big)\,.\end{aligned} \quad (40)$$

By estimates (33) and (38) the right hand side in (40) is zero and this happens for any $\epsilon>0$. We obtain therefore that for any limiting measure $\mathcal{P}^*$ we have

$$\begin{aligned}\mathcal{P}^*\Big(\pi\,:\,&\int_\Lambda f(w)d\pi(w)-\int_\Lambda f(0)d\pi(0)\\&-\int_0^w\Big[\partial_s f(s)+\int_\Lambda\alpha\nabla\cdot\Big(\mathbb{Q}\nabla f(s)\Big)\Big]\,d\pi(s)=0\,,0\le w\le t\Big)=1\,.\end{aligned}$$

Uniqueness: In the above steps we proved that any possible limit point $\mathcal{P}^*$ of a converging subsequence in $\mathcal{P}_N$ gives full measure to elements $\pi \in D([0,t],\mathcal{M}^+)$ such that: $\pi(0) = \rho_0(x)dx$ (this follows by the assumption on the initial condition), for any $s \in [0,t]$ $\pi(s) \in \mathcal{M}^+$ is absolutely continuous $\pi(s) = \pi(s,x)dx$ and with total finite mass given by $\int_\Lambda \rho_0(x)dx$ (this follows by the conservative nature of the dynamics and the initial condition), and finally for any test function f that is C^1 in time and C^2 in space we have

$$\int_\Lambda f(t)d\pi(t) - \int_\Lambda f(0)d\rho_0 - \int_0^t ds \int_\Lambda \left[\partial_s f(s) + \alpha\nabla\cdot(\mathbb{Q}\nabla f(s))\right] d\pi(s) = 0\,. \tag{41}$$

Let us now show that there is a unique $\pi(s,x)dx$ with $\pi(s) \in L^1(\Lambda)$ satisfying (41). If π_1, π_2 are two solutions, from (41) we readily obtain for $\pi = \pi_1 - \pi_2$

$$\int_0^t ds \int_\Lambda \{\partial_s f(s) + \alpha\nabla\cdot(\mathbb{Q}\nabla f(s))\} d\pi(s) = 0\,,$$

where f is the solution to the Cauchy problem

$$\begin{gathered}\partial_s f + \alpha\nabla\cdot(\mathbb{Q}\nabla f) = g,\, x \in \mathbb{R}^d, 0 < s < t,\\ f(t,x) = 0,\, x \in \mathbb{R}^d.\end{gathered}$$

Here $g \in C^1([0,t]\times\mathbb{R}^d)$ is Λ–periodic, as well as all other functions, and vanishes near $s = t$. The existence of f in the class above follows from classical results ([20] chapter 4 Section 5). Then we get in fact

$$\int_0^t ds \int_\Lambda g(s)d\pi(s) = 0\,,$$

for all g as above, yielding therefore $\pi = 0$.

We conclude therefore that any possible limiting measure $\mathcal{P}^*$ needs necessarily to be $\delta_{\rho(\cdot)}$ where $\rho(\cdot)$ is the unique weak solution to (24). Since any possible converging subsequence is converging to the same limiting measure we have that the whole sequence $\mathcal{P}_N$ is converging to $\delta_{\rho(\cdot)}$.

The convergence in probability (23) can be deduced since any weak solution of the hydrodynamic equation is weakly continuous in t i.e. it is an element of $C([0,t],\mathcal{M}^+(\Lambda))$.

Remark 1 Since we are considering a system of independent particles it would be possible to obtain an alternative proof under some special initial conditions. In particular in the case when the initial condition is obtained with identical particles distributed independently. Note that Theorem 1 covers much more general initial conditions. In this special case, the collective behavior of the occupation variables can be deduced by the scaling behavior of one single particle. We could however not find a specific reference for the scaling limit of one single IRW.

Remark 2 We consider particles evolving on a lattice but our analysis suggests that a similar geometric interpretation holds for particles jumping on the continuous space, i.e. the single particle jumps on $\mathbb{R}^d$ with a transition kernel $k(x,y)dy$ from x to dy. Lemma 1 can be generalized and any reversible kernel can be written as $\alpha(x)s(x,y)dy$ where s is symmetric in the arguments. In the inhomogeneous case $s(x,y)$ should be obtained suitably discretizing symmetrically the inhomogeneity on the jump segment $[x,y]$. We expect that Fick's law is obtained in the scaling just in the case that the site inhomogeneity α si constant. This is exactly what happens in the one–dimensional example in [17] Chapt. XI, Sec. 3.

4 Miscellany

In this section we collect some interesting remarks on the behavior of the system studied above.

4.1 Comparison between Fick and Fokker–Planck evolution

We illustrate numerically the behavior of the SIRW and EIRW stochastic models for many particles in connection with the Fokker–Planck and Fick diffusion equations with the diffusion coefficients

$$D(z) = -\frac{1}{2}\cos(2\pi z) + \frac{3}{2} \quad 0 \le z \le 1 \tag{42}$$

and

$$D(z) = \begin{cases} 2 + \tanh(50(z-0.2)) & z \le 0.5 \\ 2 - \tanh(50(z-0.8)) & z > 0.5 \end{cases} . \tag{43}$$

Note that (42) defines a $C^2([0,1])$ diffusion coefficient, whereas (43) satisfies this condition only approximatively.

The SIRW and the EIRW process are defined on $V = 0, 1, \ldots, N$ with periodic boundary conditions for M indistinguishable and independent particles. The jump rates are obtained by discretizing the diffusion coefficient D as follows. We let $z_x = x/N$ so that $z_x \in [0,1]$ and set $\alpha(x) = D(z_x)$ for $x \in V$ for the SIRW and $Q(\{x, x+1\}) = D((z_x + z_{x+1})/2)$ for the EIRW process for for $x \in V$ with $\{N, N+1\}$ identified with $\{N, 0\}$.

The numerical solution of Fokker–Planck and Fick problems with diffusion coefficients (42) and (43) are reported in Figures 2 and 3. The numerical solution was found using the NDSolve routine in Mathematica. The initial condition is $u_0(z) = 6z(1-z)$ in all simulations. We did not use a constant profile as initial condition, since that would have been the stationary solution of the Fick diffusion process so that no dynamics would have been observed. Note that in the case (43), which mimics a discontinuous diffusion coefficient, the Fick diffusion problem has a constant profile as stationary solution, whereas

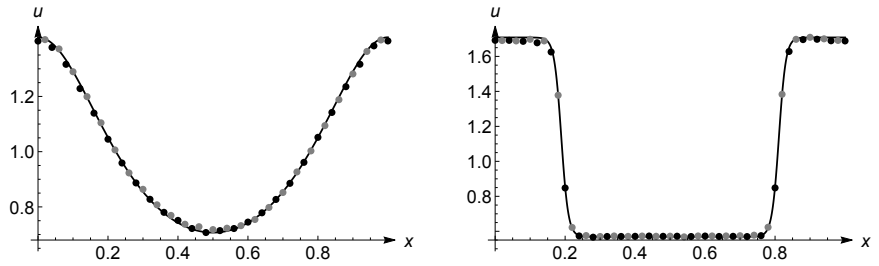

Fig. 1 Comparison between the stationary particle profile of the Random Walk problem multiplied times N/M and the stationary solution of the Fokker–Planck problem with diffusion coefficient (42) on the left and (43) on the right. The black curve is the stationary solution of the Fokker–Planck problem with initial condition $u_0(z) = 6z(1-z)$, yielding a unitary total mass. Black and gray dots report the stationary state of the corresponding Random Walk problem with two different initial states: a parabolic distribution proportional to the one used for the continuous model (black) and a uniform initial distribution (gray). The Random Walk has been run on the lattice with $N = 101$ with $M = 10041$ (black) and $M = 10100$ (gray).

the Fokker–Planck problem tends to a profile rapidly varying in correspondence of the diffusion coefficient "discontinuities".

The stationary solutions of the Fick and Fokker–Planck equations can be derived explicitly. In the Fokker–Planck case we have that at stationarity $(Du)'$ must be constant. But, for mass conservation, it must indeed be equal to zero, so that at stationarity $u(z) = c/D(z)$ where the constant c is such that

$$\int_0^1 \frac{c}{D(z)}\,\mathrm{d}z = \int_0^1 u_0(z)\,\mathrm{d}z \tag{44}$$

where, we recall, u_0 denotes the initial condition. In the Fick case we have that at stationarity Du' must be constant. But, for mass conservation, it must indeed be equal to zero, so that the stationarity solution is the constant $\int_0^1 u_0(z)\,\mathrm{d}z$.

We now compare the evolution of the SIRW process introduced in Section 2 to that of the Fokker–Planck diffusion equation on $[0,1]$. The stationary profile can be discussed explicitly, indeed, in Section 2.3 we have stated that at stationarity the average number of particles at site $x \in V$ is $b/\alpha(x) = b/D(z_x)$ with b such that

$$\sum_{x=0}^{N} \frac{b}{D(z_x)} = M \tag{45}$$

where, we recall, M is the total number of particles. Comparing (44) and (45) we have that, for N large, $b \approx c/N$. Hence, for N large the stationary particle density profiles $(b/\alpha(x))/(1/N)$ of the SIRW process is a very good approximation of the Fokker–Planck stationary solution $c/D(z)$.

For the time dependent results we simulate the stochastic model as follows: recalling that $\eta_x(t)$ is the number of particles at site x and time t, we extract an exponential random time τ with parameter $\sum_{x=0}^{N} 2\alpha(x)n_x(t)$ and set the

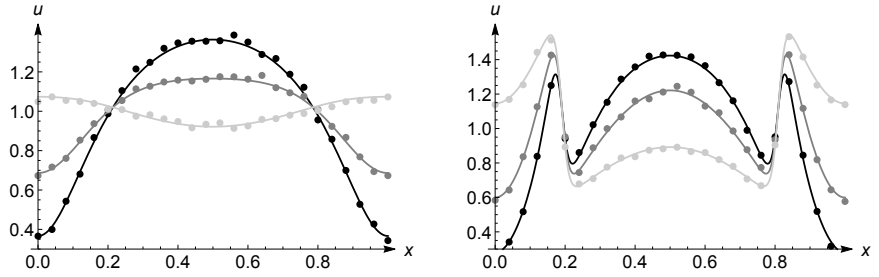

Fig. 2 Comparison between the particle profile of the Random Walk problem multiplied times N/M and the solution of the Fokker–Planck problem with diffusion coefficient (42) on the left and (43) on the right. Black, gray, and light gray curves and dots refer respectively to times $0.003005, 0.009221, 0.022273$ (left) and $0.001967, 0.006207, 0.015688$ (right). Solid curves are the solution of the Fokker–Planck problem with initial condition $u_0(z) = 6z(1-z)$, yielding a unitary total mass. Black and gray dots report the states of the corresponding Random Walk problem with the same initial condition. The Random Walk has been run on the lattice with $N = 101$ and $M = 10041$.

time equal to $t+\tau$. We associate the probability $2\alpha(y)n_y(t)/\sum_{x=0}^{N} 2\alpha(x)n_x(t)$ to each site $y \in V$ and select at random a site according to such a distribution. We move a particle from the selected site to one of the two adjacent sites with probability $1/2$.

To compute the stationary particle profile we let the system evolve for 10^3 full sweeps (in one sweep M particles are moved). Then, we average the value of the number of particles occupying each site of the lattice by considering one configuration each 10 sweeps. The numerical experiment is stopped after about 10^5 more sweeps.

In Figure 1 we compare the stationary solution of the Fokker–Planck diffusion processes with the stationary particle profile of the Random Walk. The stationary particle profile is divided times the spacing $1/N$ to get the stationary particle density profile and is divided times M since the Fokker–Planck diffusion equation has been solved with an initial state having total mass equal to one.

In Figure 2 we compare the evolution of the Fokker–Planck diffusion processes with the Random Walk particle profile. As for the stationary state, the Random Walk particle profile has been divided times the spacing $1/N$ to get the particle density profile and divided times M since the Fokker–Planck diffusion equation has been solved with an initial state having total mass equal to one. Moreover, the time measured in the stochastic evolution has been divided times N^2. Averages have been computed by considering 50 independent realizations of the process and averaging the particle distribution at equal times.

Finally, we compare the evolution of the EIRW process introduced in Section 2 to that of the Fick diffusion equation on $[0, 1]$. In this case the stationary state is trivial, indeed, we compute the stationary particle distribution profile as outlined for the SIRW case and we find that it is constant with very high precision.

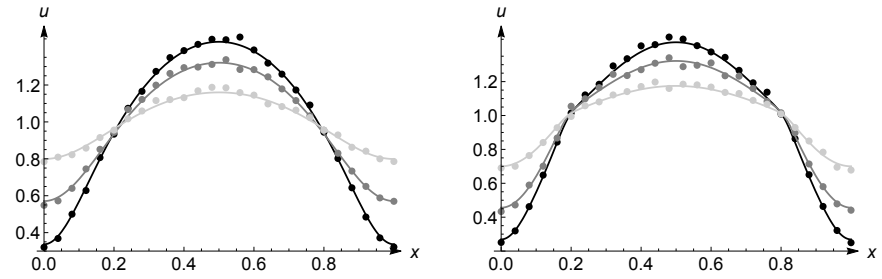

Fig. 3 Comparison between the particle profile of the Random Walk problem multiplied times N/M and the solution of the Fick problem with diffusion coefficient (42) on the left and (43) on the right. Black, gray, and light gray curves and dots refer respectively to times $0.002991, 0.009102, 0.021696$ (left) and $0.001916, 0.005856, 0.014081$ (right). Solid curves are the solution of the Fick problem with initial condition $u_0(z) = 6z(1-z)$, yielding a unitary total mass. Black and gray dots report the states of the corresponding Random Walk problem with the same initial condition. The Random Walk has been run on the lattice with $N = 101$ and $M = 10041$.

For the time dependent results we simulate the stochastic model as follows: recalling $\eta_x(t)$ is the number of particles at site x and time t, we extract an exponential random time τ with parameter $\sum_{x=0}^{N}(Q(\{x-1,x\}) + Q(\{x,x+1\}))\eta_x(t)$ and set the time equal to $t+\tau$. We associate the probability $(Q(\{y-1,y\}) + Q(\{y,y+1\}))\eta_y(t)/\sum_{x=0}^{N}(Q(\{x-1,x\}) + Q(\{x,x+1\}))\eta_x(t)$ to each site $y \in V$ and select at random a site according to such a distribution. We move a particle from the selected site, say y, to the left with probability $Q(\{y-1,y\})/(Q(\{y-1,y\})+Q(\{y,y+1\}))$ and to the right with probability $Q(\{y,y+1\})/(Q(\{y-1,y\}) + Q(\{y,y+1\}))$.

In Figure 3 we compare the evolution of the Fick diffusion processes with the Random Walk particle profile. As for the stationary state, the Random Walk particle profile has been divided times the spacing $1/N$ to get the particle density profile and divided times M since the Fick diffusion equation has been solved with an initial state having total mass equal to one. Moreover, the time measured in the stochastic evolution has been divided times N^2. Averages have been computed by considering 50 independent realizations of the process and averaging the particle distribution at equal times.

4.2 Einstein relation

A very general modelization of the presence of an external field is obtained perturbing the rates as follows. Let $\phi : \Lambda \to \mathbb{R}^d$ be a smooth vector field that acts on particles. The action of the field is encoded in the perturbed transition rates that are defined as

$$c^{\phi}_{x,y}(\eta) := c_{x,y}(\eta) e^{\phi_N(x,y)}\,, \tag{46}$$

where ϕ_N is the discretization (11) of the vector field. Rates that correspond to movements of the particles with an associate positive work of the field are

enhanced while instead rates that correspond to movements of the particles with an associate negative work of the field are decreased.

Let us first discuss the influence of an external field in the case of spatially homogeneous models [2]. The hydrodynamic scaling limit of diffusive particle systems under the action of a weakly asymmetric external field is associated to equations of the form

$$\partial_t \rho = \nabla \cdot (\mathbb{D}(\rho)\nabla\rho) - 2\nabla \cdot (\mathbb{M}(\rho)\phi) \ . \tag{47}$$

The symmetric and positive definite matrix $\mathbb{D}$ is the diffusion matrix while the symmetric and positive definite matrix $\mathbb{M}$ is the mobility matrix. For independent particles we have that the diffusion matrix coincides with the identity matrix $\mathbb{D} = \mathbb{I}$ while instead $\mathbb{M} = \rho\mathbb{I}$.

In the homogeneous case a relevant thermodynamic relationship is the so called Einstein relation between the diffusion matrix and the mobility given by

$$\mathbb{D}(\rho) = \mathbb{M}(\rho) f''(\rho)\,, \tag{48}$$

that says that the two matrices $\mathbb{D}$ and $\mathbb{M}$ are proportional and the proportionality factor is the second derivative of the density of free energy f (that is $f(\rho) = \rho\log\rho$ in the independent particles case as discussed after (17)).

Let us now move to the spatial inhomogeneous case. An interesting way of writing the hydrodynamic equation (24) is obtained computing the gradient appearing there, getting

$$\partial_t \rho = \nabla \cdot (\alpha\mathbb{Q}\nabla\rho) + \nabla \cdot (\alpha\rho\mathbb{Q}\nabla\log\alpha) \ .$$

It is very natural to interpret this equation introducing the space dependent diffusion matrix $\mathbb{D}(x,\rho) = \alpha(x)\mathbb{Q}(x)$ and the space dependent mobility matrix $\mathbb{M}(x,\rho) = \alpha(x)\rho(x)\mathbb{Q}(x)$. Note that they satisfy the Einstein relation for each $x \in \Lambda$. Indeed recalling that the density of free energy is $f(\rho) = \rho\log\rho$ for independent particles we have

$$\mathbb{D}(x,\rho) = \mathbb{M}(x,\rho) f''(\rho)\,, \qquad \forall x \in \Lambda\ , \forall \rho\,.$$

With this identification we have that the inhomogeneity determines space dependent diffusion and mobility matrices. The form of these matrices depend both on the weights on the edges and on the weights on the vertices. The spatial inhomogeneity of the material generates however also an external field that depends just on the site inhomogeneity. This external field is exactly $-(1/2)\nabla\log\alpha$.

We show that this interpretation is correct. This is done switching on a weak external field and showing that the hydrodynamic equation is modified with the appearance of a term proportional to the mobility matrix $\mathbb{M}(x,\rho)$ like in the homogeneous case (47). In presence of an external field the rates are modified according to (46) and correspondingly the instantaneous current becomes

$$j^{\phi}_{\eta}(x,y) = c_{x,y}(\eta)e^{\phi_N(x,y)} - c_{y,x}(\eta)e^{\phi_N(y,x)} \ . \tag{49}$$

Recall that the values of ϕ_N are infinitesimal (11) so that we have

$$e^{\phi_N(x,y)} = 1 + \phi_N(x,y) + o(1/N)\,.$$

The instantaneous current is therefore

$$j^{\phi}_{\eta}(x,y) = j_{\eta}(x,y) + (c_{x,y}(\eta) + c_{y,x}(\eta))\,\phi_N(x,y) + o(1/N)\,. \tag{50}$$

Substituting (50) to j_η in the second term in (29) and ignoring negligible terms we obtain the extra factor

$$\frac{1}{N^d}\sum_{x\in\Lambda_N}\int_0^t ds\,\alpha(x)\eta_s(x)\Big[N^2\sum_{y\in C(x)} Q(\{x,y\})(f(s,y)-f(s,x))\phi_N(x,y)\Big]\,.$$

With computations similar to the ones in the proof of Theorem 1 we have that the term inside squared parenthesis in the above formulas coincides up to uniform infinitesimal terms with

$$2\mathbb{Q}(x)\phi(x)\cdot\nabla f(x,s)\,.$$

This means that the hydrodynamic equation in presence of a weak external field becomes

$$\partial_t\rho = \nabla\cdot(\mathbb{D}(x,\rho)\nabla\rho) - 2\nabla\cdot\left(\mathbb{M}(x,\rho)\left(\phi - \frac{1}{2}\nabla\log\alpha\right)\right)\,.$$

We deduce that $\mathbb{M}(x,\rho)$ plays the role of the mobility matrix and we obtain a version of the Einstein relation in the non–homogeneous framework.

4.3 Reversible diffusions

As we observed in the previous section, in the case of independent particles the hydrodynamic equation describing the collective behavior of several particles is linear and coincides with the equation of the evolution of the probability distribution of one single particle. Since the scaling limit of one single particle is a diffusion process and since our discrete models are reversible it is natural to compare the class of hydrodynamic equations that we obtained with the possible Fokker Plank equations associated to reversible diffusions.

At the microscopic level we obtained that the reversibility condition has a geometric interpretation. We have indeed that the models are reversible if and only if the rates are chosen according to some weights associated to the edges and the vertices of the graph (see Lemma 1). In the case of continuous diffusion process we have a similar geometric characterization of reversibility, indeed reversible diffusions can be parameterized by a positive function and a symmetric and positive definite matrix, that can be interpreted as the metric tensor. These are the continuous counterparts of the discrete weights on the graph.

We refer to [15, 17] for the basic facts about diffusion processes. For simplicity we consider the processes on $\mathbb{R}^d$ instead that on the torus. Consider a diffusion process of the form

$$dX_t = A(X_t)dt + \mathbb{B}(X_t)dW_t \tag{51}$$

where $A = (A_1(x), \dots, A_d(x))$ is a smooth vector field, $\mathbb{B}(x)$ is a $d \times d$ matrix smoothly depending on x and $W = (W_1, \dots . W_d)$ is a d dimensional standard Brownian motion. The corresponding Fokker Plank equation describing the evolution of the probability distribution is given by

$$\partial_t \rho = \nabla \cdot [-\rho A + C] \tag{52}$$

where

$$C_i = \frac{1}{2} \sum_{j=1}^{d} \partial_{x_j} \left(\rho \left(\mathbb{B}\mathbb{B}^T \right)_{i,j} \right) , \qquad i = 1, \dots, d \, .$$

Note that while in the equation (51) appears the matrix $\mathbb{B}$, the evolution of the probability distribution depends just on the symmetric matrix $\mathbb{B}\mathbb{B}^T$. The condition of reversibility (see [15, 17]) is that the vector

$$F_i := \sum_{k=1}^{d} (\mathbb{B}\mathbb{B}^T)^{-1}_{i,k} \left[2A_k - \sum_j \partial_{x_j} (\mathbb{B}\mathbb{B}^T)_{k,j} \right] , \qquad i = 1, \dots, d \, , \tag{53}$$

is of gradient type. In this case, under additional confinements assumptions, the stationary solution of the Fokker Planck equation is

$$\bar{\rho}(x) = \frac{e^{-\psi(x)}}{Z}$$

where $F = -\nabla \psi$. We have therefore that all the reversible diffusion processes can be parameterized in terms of the function ψ and the symmetric and positive definite matrix $\mathbb{B}\mathbb{B}^T$. This is because you can fix arbitrarily these two objects and then A is completely determined by (53). If we use instead the positive function α related to ψ by $\psi = \log \alpha$ and the symmetric positive definite matrix $\mathbb{Q}(x) = \mathbb{B}\mathbb{B}^T(x)\alpha^{-1}(x)/2$ we have that the Fokker Plank equation (52) is given by

$$\partial_t \rho = \nabla \cdot (\mathbb{Q} \nabla (\alpha \rho)) \tag{54}$$

that is exactly of the type of our hydrodynamic equation (24). It is important to note however that in (24) the matrix $\mathbb{Q}$ has to be diagonal while instead this is not the case in (54). As we will discuss in the next section this is due to the special lattice that we are considering in Theorem 1. We can obtain non diagonal matrices considering different lattices.

4.4 Different lattices

Here we show that we obtained just equations with diagonal matrices $\mathbb{Q}$ since we are considering a squared lattice. We briefly discuss how to handle different situations obtaining non diagonal matrices $\mathbb{Q}$. From the proof of Theorem (1) we known that the basic computation to identify the limiting equation is to approximate up to uniformly infinitesimal corrections the term inside square parenthesis in (30) that is

$$N^2 \sum_{y \in C(x)} Q(\{x,y\}) \left(f(s,x) - f(s,y)\right) . \tag{55}$$

The generalized framework that we consider now is a lattice having vertices coinciding again with Λ_N but having more edges than the usual square lattice. This corresponds to allowing more possible jumps to the particles. The graph on which the particles are evolving is obtained as follows. We start with $\mathbb{Z}^d$ with more edges with respect to the usual ones that are connecting just the minimal distance vertices. The collection of directed edges exiting form any vertex $x \in \mathbb{Z}^d$ are of the form $(x, x+\tilde{v}^i)$ where $\tilde{v}^i$ for $i = 1, \dots, k$ is a collection of vectors such that $x + \tilde{v}^i \in \mathbb{Z}^d$. Since we are always requiring that an unoriented edge can be crossed on both directions then k has to be necessarily an even number and for any vector $\tilde{v}^i$ there should be a corresponding label j such that $\tilde{v}^j = -\tilde{v}^i$ so that both $(x, x+\tilde{v}^i)$ and $(x+\tilde{v}^i, x)$ are elements of the directed edges E_N. The lattice that we consider is obtained scaling by a factor of N^{-1} this lattice. In particular we call $v^i := N^{-1}\tilde{v}^i$.

We have therefore that on each lattice site $x \in \Lambda_N$ there are k different edges incident that correspond to k possible jumps of one particle from x to $x + v^j$, $j = 1, \dots, k$. In the case of the square lattice we had $k = 2d$ and each v^j is equal to $\pm e^i$ for some i. Note that we have now $|C(x)| = k$. More general frameworks are of course possible but for simplicity we restrict to this generalization.

We need to give weights to the vertices and the edges of the lattice suitably discretizing smooth objects. The weights on the vertices are associated as before computing a smooth function α on the corresponding point. For the edges we need to generalize the construction done before.

We consider a smooth metrics $\mathcal{Q}(x)$ that is a symmetric and positive definite $d \times d$ matrix depending in a regular way (C^2 for example) on the continuous variable $x \in \Lambda$. We associate the weight to an edge of the form $\{x, x+v^i\}$ as

$$Q(\{x, x+v^i\}) := \tilde{v}^i \cdot \mathcal{Q}(x + v^i/2)\tilde{v}^i =: Q^i(x + v^i/2) . \tag{56}$$

The appearance of the $\tilde{v}^i$ vectors above is due to the fact that we have $|v^i| \sim 1/N$ (since the vectors without tilde are comparable with the mesh of the lattice) and we want that the weights to be associated to the edges are not infinitesimal in N but are of order one. The last equality in (56) is just the definition of a shorthand for the weights. With a suitable Taylor expansion we

get that (55) coincides up to uniformly infinitesimal terms with

$$N^2 \sum_{i=1}^{k} \left(Q^i(x) + \nabla Q^i(x) \cdot \frac{v^i}{2} \right) \left(\nabla f(x) \cdot v^i + \frac{1}{2} v^i \cdot H(x) v^i \right) , \qquad (57)$$

where $H(x)$ is the Hessian matrix at x of the function f having elements $(H(x))_{l,m} = \partial_{x_l} \partial_{x_m} f(x)$.

Recall that k is an even number ad if v^i is the vector associated to a possible jump then also $-v^i$ is a vector associated to a possible jump. Due to this, we have that the leading term in the product in (57) that is

$$N^2 \sum_{i=1}^{k} Q^i(x) \nabla f(x) \cdot v^i \qquad (58)$$

is identically zero. This is because we can pair the edges exiting from x in such a way that if the label i is paired to the label j then $v^i = -v^j$ and consequently $Q^i(x) = Q^j(x)$. Of the remaining three terms obtained when we develop the product in (57) we have that one is infinitesimal. The two relevant ones that survive are

$$\frac{1}{2} \sum_{i=1}^{k} Q^i(x) N v^i \cdot H(x) N v^i + \frac{1}{2} \sum_{i=1}^{k} \left(\nabla Q^i(x) \cdot N v^i \right) \left(\nabla f(x) \cdot N v^i \right) .$$

The above expression coincides up to uniform infinitesimal terms with

$$\nabla \cdot (\mathbb{Q}(x) \nabla f(x))$$

where the matrix $\mathbb{Q}$ is defined as

$$\mathbb{Q}_{l,m}(x) = \frac{1}{2} \sum_{i=1}^{k} Q^i(x) \tilde{v}^i_l \tilde{v}^i_m . \qquad (59)$$

With the same arguments of the proof of Theorem 1, but using this expansion, we can prove that the limiting equation is again of the form (24) but the matrix $\mathbb{Q}$ is given by (59) that in general is non–diagonal.

4.5 Uphill currents

A current is said to move "uphill" when particles migrate *up the gradient*, namely towards regions of higher concentration, thus violating the basic tenets of Fick's law of diffusion. The onset of such uphill currents can be traced back to the action of an external field, to the presence of mutual interactions in a multi-component system or, for single-component systems, to a phase transition, and was recently investigated in a variety of lattice gas models, cf. Refs [5, 9–12].

We look, here, at the case where two inhomogeneous diffusion processes take place in two intervals of length $L > 0$, for two concentration functions v,

u, being connected by conditions of equality of concentration and of flux at the two endpoints. The latter is meant in the sense that the outflux of v equals the influx of u. However, v solves Fick's equation, while u solves a Fokker-Planck type equation. The diffusivities are assumed to be piecewise constant.

We consider the stationary case, see also Refs. for a more general discussion about the observation of uphill currents.

Thus the problem is, in a distributional formulation,

$$-(Kv_x)_x = 0\,, \qquad 0 < x < L\,, \tag{60}$$
$$-(Du)_{xx} = 0\,, \qquad 0 < x < L\,, \tag{61}$$
$$v(0) = u(0)\,, \tag{62}$$
$$v(L) = u(L)\,, \tag{63}$$
$$Kv_x(0) = -Du_x(0)\,, \tag{64}$$
$$Kv_x(L) = -Du_x(L)\,. \tag{65}$$

Here

$$K(x) = K_1\chi_{(0,b)}(x) + K_2\chi_{(b,L)}(x)\,, \tag{66}$$

and

$$D(x) = D_1\chi_{(0,a)}(x) + D_2\chi_{(a,L)}(x)\,, \tag{67}$$

for given positive constants K_i, D_i, and for b, $a \in (0, L)$.

We assume here $D_1 \neq D_2$; see also Remark 3.

We refer to the following weak formulation of this problem: find $v \in H^1(0, L)$, $u \in L^\infty(0, L)$ such that $Du \in H^1(0, L)$ and

$$\int_0^L \{Kv_x\zeta_x + (Du)_x\eta_x\}dx = 0\,, \tag{68}$$

for all ζ, $\eta \in C^1([0, L])$ such that $\zeta(0) = \eta(0)$ and $\zeta(L) = \eta(L)$. Here $H^1(0, L)$ is the standard space of square integrable functions with square integrable Sobolev derivative, which is known to be embedded in $C([0, L])$. Then, also using our assumptions on D, we impose (62) and (63) in a classical pointwise sense.

It follows from straightforward reasoning and from (68) that Kv_x and $(Du)_x$ are constant in $(0, L)$. Thus invoking the definitions of K and D, we recover in the classical sense

$$-v_{xx} = 0\,, \qquad \text{in } (0, b) \cup (b, L), \tag{69}$$
$$v(b-) = v(b+)\,, \tag{70}$$
$$K_1v_x(b-) = K_2v_x(b+)\,, \tag{71}$$

and

$$-u_{xx} = 0\,, \qquad \text{in } (0, a) \cup (a, L), \tag{72}$$
$$D_1u(a-) = D_2u(a+)\,, \tag{73}$$
$$D_1u_x(a-) = D_2u_x(a+)\,. \tag{74}$$

Note that more generally one should write e.g., (74) as

$$(D_1 u)_x(a-) = (D_2 u)_x(a+)\,.$$

but this is not relevant under our assumption of piecewise constant D. A similar remark applies to (64), (65), which indeed are valid in a pointwise sense.

Clearly problem (60)–(65) is invariant for multiplication by a constant, and always has the null solution. Therefore for the sake of precision we'll impose also the following normalization condition

$$v(0) = 1\,. \tag{75}$$

The formulation (69)–(71) yields immediately

$$v(x) = \begin{cases} v_x(b-)(x-b) + v(b-)\,, & 0 < x < b\,, \\ \dfrac{K_1}{K_2} v_x(b-)(x-b) + v(b-)\,, & b < x < L\,. \end{cases} \tag{76}$$

Instead the formulation (72)–(74) implies

$$u(x) = \begin{cases} u_x(a-)(x-a) + u(a-)\,, & 0 < x < a\,, \\ \dfrac{D_1}{D_2} u_x(a-)(x-a) + \dfrac{D_1}{D_2} u(a-)\,, & a < x < L\,. \end{cases} \tag{77}$$

The normalization condition and (62) lead to

$$-v_x(b-)b + v(b-) = 1\,, \tag{78}$$

$$-u_x(a-)a + u(a-) = 1\,, \tag{79}$$

while (63) gives

$$\frac{K_1}{K_2} v_x(b-)(L-b) + v(b-) = \frac{D_1}{D_2} u_x(a-)(L-a) + \frac{D_1}{D_2} u(a-)\,. \tag{80}$$

Finally both (64) and (65) are equivalent to

$$K_1 v_x(b-) = -D_1 u_x(a-)\,. \tag{81}$$

Thus we have a linear system (78)–(81) of 4 equations in the 4 unknowns $v(b-)$, $v_x(b-)$, $u(a-)$, $u_x(a-)$.

Its solution is

$$\begin{aligned} v(b-) &= \frac{(D_1K_2 - D_2K_1)b + K_1(D_2+K_2)L}{D_2(K_2-K_1)b + K_1(D_2+K_2)L} \\ &= 1 + \frac{K_2(D_1-D_2)b}{D_2(K_2-K_1)b + K_1(D_2+K_2)L}\,, \\ v_x(b-) &= \frac{K_2(D_1-D_2)}{D_2(K_2-K_1)b + K_1(D_2+K_2)L}\,, \\ u(a-) &= 1 + \frac{1}{D_1}\,\frac{K_1K_2(D_2-D_1)a}{D_2(K_2-K_1)b + K_1(D_2+K_2)L}\,, \\ u_x(a-) &= \frac{1}{D_1}\,\frac{K_1K_2(D_2-D_1)}{D_2(K_2-K_1)b + K_1(D_2+K_2)L}\,, \end{aligned}$$

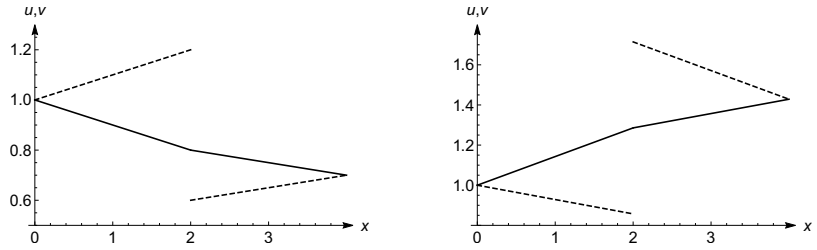

Fig. 4 Functions v (continuous line) and u (dashed line) for $L = 4$, $b = a = 2$, $K_1 = 1$, and $K_2 = 2$ with $D_1 = 1$ and $D_2 = 2$ on the left and $D_1 = 2$ and $D_2 = 1$ on the right.

provided

$$D_2(K_2 - K_1)b + K_1(D_2 + K_2)L \neq 0\,.$$

But

$$D_2(K_2 - K_1)b + K_1(D_2 + K_2)L = D_2K_2b + K_1K_2L + K_1D_2(L - b) > 0\,,$$

since $L > b$.

We remark that each one of $v_x(x)$, $x \neq b$, and $u_x(x)$, $x \neq a$, has constant sign; the two signs always differ. This remark does not imply that u is monotonic, in view of its discontinuous character.

We may also compute

$$v(L) = u(L) = 1 + (D_1 - D_2)\frac{(K_2 - K_1)b + K_1L}{D_2(K_2 - K_1)b + K_1(D_2 + K_2)L} > 0\,,$$

where the last inequality follows from elementary reasoning.

Remark 3 If $D_1 = D_2$ one can see easily that the solution is flat, that is $v(x) = u(x) = 1$ for all $x \in (0, L)$. This is a special case of next Remark 4.

Instead the relative values of K_1, K_2 do not seem to play any special role.

Remark 4 If one assumes for u a Ficksian equation similar to the one solved by v, it follows immediately that $v(x) = u(x) = 1$ for all $x \in (0, L)$: indeed since both v and u are continuous and piecewise linear, and then monotonic, they share their minimum and maximum values, at the endpoints. But there their fluxes are opposite in sign, and must therefore actually vanish, yielding the claim.

Remark 5 If we replace the conditions (62), (63) with the partition type balances

$$v(0) = Du(0)\,, \tag{82}$$
$$v(L) = Du(L)\,, \tag{83}$$

it can be immediately seen that setting $\tilde{u} = Du$ we obtain for v, $\tilde{u}$ a problem with two equations of Fick type; more exactly we are in the case of Remark 4 with the diffusivity in the equation for $\tilde{u}$ being identically 1. Then we have

$$v(x) = 1\,, \qquad D(x)u(x) = 1\,, \qquad x \in (0, L)\,. \tag{84}$$

On the other hand, conditions (82) are comparable to (73); that is they are the conditions we would expect if the whole system was subject to the equation

$$-(K(x)(D(x)U(x))')' = 0\,,$$

with the suitable choices of K, D.

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