SAPIENZA
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Microscopic models for Fick and Fokker-Planck diffusion equations

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The problem

Propose microscopic models to derive Fick and Fokker–Planck diffusion laws.

Motivation:

- study diffusion in presence of space inhomegeneities;
- in applied sciences two different macroscopic equations are used: the Fick and the Fokker–Planck equations;
- give e microscopic interpretations of the two macroscospic equations;
- relate the macroscopic behavior to the microscopic structure of the space inhomogeneities.

Bibliography

[1] D. Andreucci, E.N.M. Cirillo, M. Colangeli, D. Gabrielli, “Fick and Fokker-Planck diffusion law in inhomogeneous media.” *Journal of Statistical Physics* **174**, 469–493 (2019).

[2] M.J. Schnitzer, *Theory of continuum random walks and application to chemotaxis.* Physical Review E **48**, 2553–2568 (1993).

[3] P.T. Landsberg, *$D\,grad\,v$ or $grad(Dv)$?* Journal of Applied Physics **56**, 1119 (1984).

[4] F. Sattin, *Fick's law and Fokker–Planck equation in inhomogeneous environments.* Physics Letters A **372**, 3921–3945 (2008).

[5] P. Lançon, *Drift without flux: Brownian walker with a space dependent diffusion coefficient.* Europhysics Letters **54**, 28 (2001).

[6] .... wide literature in the framework of stochastic partial differential equations ....

Macroscopic equations

The Fick law for space homogeneous systems

Matter diffuses in the region $\Omega \subset \mathbb{R}^3$ and $u(x,t)$ is the density inside Ω.

Matter is conserved:

$$\frac{\partial u}{\partial t} + \nabla \cdot J = 0$$

where J is the flux.

The flux is related to the density profile by the Fick's law

$$J = -D\nabla u$$

where the "constant" $D > 0$ is called *diffusion coefficient*.

Combining the two equations find the *Fick diffusion* or *heat equation*

$$\frac{\partial u}{\partial t} + \nabla \cdot (-D\nabla u) = 0 \Longrightarrow \frac{\partial u}{\partial t} = D\Delta u \ .$$

The Fick law for space inhomogeneous systems

The diffusion coefficient $D(x)$ is a function of the space variable x.

The Fick's law for the flux reads

$$J(x,t) = -D(x)\nabla u(x,t) \ .$$

Combining with the continuity equation

$$\frac{\partial u}{\partial t} + \nabla \cdot (-D\nabla u) = 0 \Longrightarrow \frac{\partial u}{\partial t} = \nabla \cdot (D\nabla u) \ ,$$

namely, the *Fick diffusion law* or *equation*.

The Fokker–Planck diffusion equation

Assume the flux is given by

$$J(x,t) = -\nabla(D(x)u(x,t)) \ ,$$

note that the two approches coincide when D is constant.

Combining with the continuity equation

$$\frac{\partial u}{\partial t} + \nabla \cdot (-\nabla(Du)) = 0 \Longrightarrow \frac{\partial u}{\partial t} = \Delta(Du) \ ,$$

namely, the *Fokker–Planck diffusion law* or *equation*.

Basic question

Which is the correct expression for the flux in presence of space inhomogeneities?

$$-D(x)\nabla u(x,t) \quad \text{or} \quad -\nabla(D(x)u(x,t))$$

P.T. Landsberg, *$D\,grad\,v$ or $grad(Dv)$?* Journal of Applied Physics **56**, 1119 (1984).

Note that

$$-\nabla(D(x)u(x,t)) = -D(x)\nabla u(x,t) - u(x,t)\nabla D(x)$$

in the Fokker–Planck case a drift term with velocity $-\nabla D$ is added to the Fick's flux.

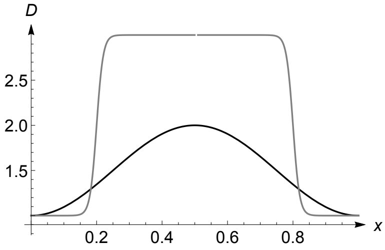
Examples in $\Omega = [0, 1]$

Consider

$$D_{\mathrm{c}}(x) = -\frac{1}{2}\cos(2\pi x) + \frac{3}{2}$$

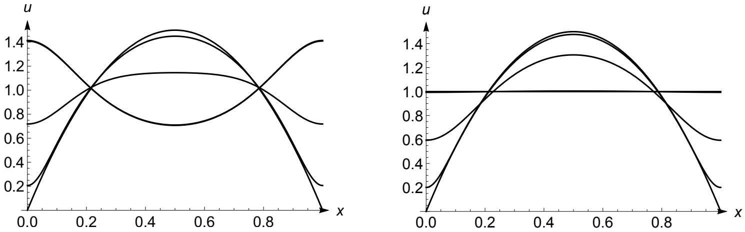
and

$$D_{\mathrm{d}}(z) = \begin{cases} 2 + \tanh(50(x - 0.2)) & x \leq 0.5 \\ 2 - \tanh(50(x - 0.8)) & x > 0.5 \end{cases} .$$



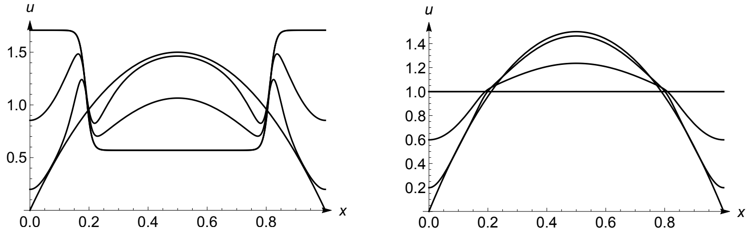
Black curve for D_{c} and gray curve for D_{d} (mimics the discontinuous case).

Examples in $\Omega = [0, 1]$



Solution of the periodic Fokker–Planck (left) and Fick (right) problem with diffusion coefficient D_{c}. The five curves report the solution at times $t = 0, 0.001, 0.01, 0.1, 1$, larger the time higher the value at the boundaries. The two curves corresponding to times 0.1 and 1 are coincident. The initial condition is $u_0(z) = 6z(1 - z)$

Examples in $\Omega = [0, 1]$



Solution of the periodic Fokker–Planck (left) and Fick (right) problem with diffusion coefficient D_{d}. The five curves report the solution at times $t = 0, 0.001, 0.01, 0.1, 1$, larger the time higher the value at the boundaries. The two curves corresponding to times 0.1 and 1 are coincident. The initial condition is $u_0(z) = 6z(1 - z)$

Remark on the stationary solution

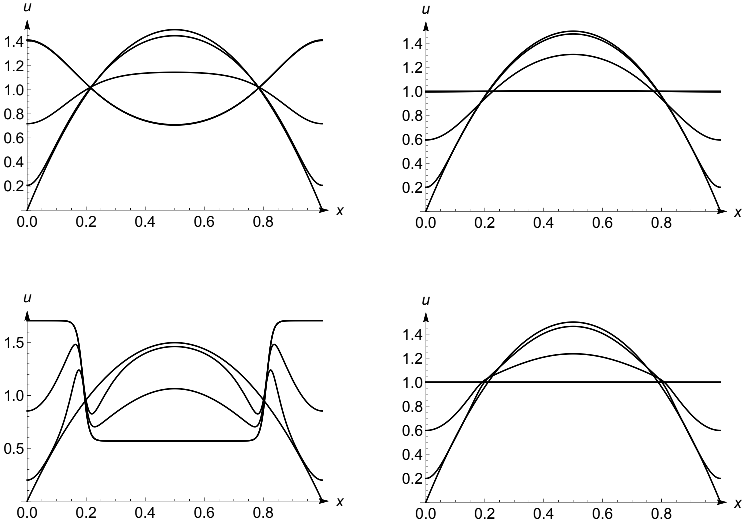
Fick

$$\cancel{\frac{\partial u}{\partial t}} = \nabla \cdot (D \nabla u) \Longrightarrow u_{\mathrm{stat}}(x) = \mathrm{const}$$

Fokker–Planck

$$\cancel{\frac{\partial u}{\partial t}} = \Delta (D u) \Longrightarrow D(x) u_{\mathrm{stat}}(x) = \mathrm{const} \Longrightarrow u_{\mathrm{stat}}(x) = \frac{\mathrm{const}}{D(x)}$$

Examples in $\Omega = [0, 1]$



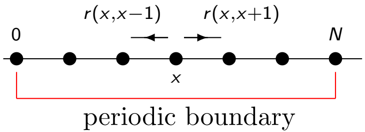
Microscopic model

Inhomogeneous Simple Random Walk

Consider a Random Walk on the graph $V = \{0, 1, \ldots, N\}$ with rates $r(x, y)$, namely,

> $r(x, y)\,\mathrm{d}t$ is the probability that the particle jumps from site x to site y in the interval of time $(t, t + \mathrm{d}t)$.

Assume the rate $r(x, y) = 0$ if x and y are not nearest neighbors, namely $y \neq x \pm 1$.



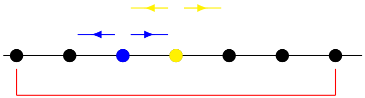
Assume that the rates have the structure

$$r(x, y) = \alpha(x) Q(\{x, y\}) \; .$$

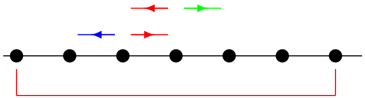
Note that this is the most general reversible random walk.

Two special cases

SIRW. Site Inhomogeneous Random Walk: $r(x,y) = \alpha(x)$, $Q = 1$.



EIRW. Edge Inhomogeneous Random Walk: $r(x,y) = Q(\{x,y\})$, $\alpha = 1$.



Schnitzer's example (1993)

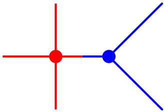
A diluted gas moves in a closed box through a dense mesh of iron wool.

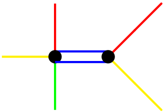
Model one: the iron wool density is uniform and the box experiences a fixed temperature gradient (the typical particle speed varies continuously throughout the box).

Model two: the temperature is uniform, but the iron wool density varies continuously in the box.

They derive Fokker–Planck for model one and Fick for model two.

Analogies with our models: model one is inhomogeneous but locally isotropic (SIRW), whereas model two is not (EIRW).





Many particles

Model for M independent and indistinguishable particles: $\eta(x)$ is the number of particles at site $x \in V$.

The rate at which one particle jumps from site x to its nearest neighbor y is

$$\eta(x)r(x,y) = \eta(x)\alpha(x)Q(\{x,y\}).$$

More formally, a configuration of particles is an element of the set $\Omega := \{\eta \in \mathbb{N}^V, \sum_{x\in V} \eta(x) = M\}$.

If x, y are neighbors and $\eta \in \Omega$ such that $\eta(x) \geq 1$, the configuration $\eta^{x,y}$ is obtained by η letting one particle jump from x to y.

The stochastic evolution is encoded by the generator

$$\mathcal{L}f(\eta) = \sum_{(x,y):\, x,y \text{ are n.n.}} c_{x,y}(\eta)\,[f(\eta^{x,y}) - f(\eta)]$$

with $c_{x,y}(\eta) = \eta(x)\alpha(x)Q(\{x,y\})$.

Construction of the dynamics in a simulation

At time t extract an exponential random time τ with parameter the total rate

$$\sum_{x=0}^{N} \alpha(x)[Q(\{x-1,x\}) + Q(\{x,x+1\})]\eta_x(t)$$

and set the time equal to $t+\tau$.

Associate to each site $y \in V$ the probability

$$\frac{\alpha(y)[Q(\{y-1,y\}) + Q(\{y,y+1\})]\eta_y(t)}{\sum_{x=0}^{N} \alpha(x)[Q(\{x-1,x\}) + Q(\{x,x+1\})]\eta_x(t)}.$$

Select at random a site according to such a distribution.

Move a particle from the selected site y to the left with probability $Q(\{y-1,y\})/(Q(\{y-1,y\}) + Q(\{y,y+1\}))$ and to the right with probability $Q(\{y,y+1\})/(Q(\{y-1,y\}) + Q(\{y,y+1\}))$.

Hydrodynamic limit for the SIRW

Set $z_x = x/N \in [0,1]$, consider a positive function $D \in C^2([a,b])$ and set $\alpha(x) = D(z_x)$ for $x \in V$.

The change of the number of particles at site x in a small interval Δt can be computed as

$$\begin{aligned} &\eta_x(t+\Delta t) - \eta_x(t) \\ &\qquad = -2\alpha(x)\eta_x(t)\Delta t + \alpha(x-1)\eta_{x-1}(t)\Delta t + \alpha(x+1)\eta_{x+1}(t)\Delta t. \end{aligned}$$

Rewrite as

$$\begin{aligned} &\frac{\eta_x(t+\Delta t) - \eta_x(t)}{\Delta t/N^2} \\ &\qquad = \frac{[\alpha(x+1)\eta_{x+1}(t) - \alpha(x)\eta_x(t)] - [\alpha(x)\eta_x(t) - \alpha(x-1)\eta_{x-1}(t)]}{1/N^2} \end{aligned}$$

Rescaling time as $t/N^2 \to t$, in the limit $N \to \infty$ the particle density $\eta_x(t)/(1/N)$ tends to a function $u(z,t)$ solving

$$\frac{\partial u}{\partial t} = \frac{\partial^2 Du}{\partial z^2} \quad \text{(Fokker–Planck)}.$$

Hydrodynamic limit for the EIRW

Let $Q(\{x,x+1\}) = D((z_x + z_{x+1})/2)$ be the rate associated with the edge $\{x,x+1\}$ for $x \in V$, where $\{N, N+1\}$ is identified with $\{N,0\}$.

The change of the number of particles at site x in a small interval Δt can be computed as

$$
\begin{aligned}
\eta_x(t+\Delta t) - \eta_x(t) \;=\; & -(Q(\{x-1,x\}) + Q(\{x,x+1\}))\eta_x(t)\Delta t \\
& +(Q(\{x-2,x-1\}) + Q(\{x-1,x\})) \\
& \quad \times \frac{Q(\{x-1,x\})}{Q(\{x-2,x-1\}) + Q(\{x-1,x\})}\eta_{x-1}(t)\Delta t \\
& +(Q(\{x,x+1\}) + Q(\{x+1,x+2\})) \\
& \quad \times \frac{Q(\{x+1,x\})}{Q(\{x,x+1\}) + Q(\{x+1,x+2\})}\eta_{x+1}(t)\Delta t
\end{aligned}
$$

Hydrodynamic limit for the EIRW

Hence

$$\eta_x(t+\Delta t) - \eta_x(t)$$
$$= -(Q(\{x-1,x\}) + Q(\{x,x+1\}))\eta_x(t)\Delta t$$
$$+ Q(\{x-1,x\})\eta_{x-1}(t)\Delta t + Q(\{x+1,x\})\eta_{x+1}(t)\Delta t \quad .$$

Rewrite

$$\frac{\eta_x(t+\Delta t) - \eta_x(t)}{\Delta t / N^2}$$
$$= \frac{Q(\{x,x+1\})[\eta_{x+1}(t) - \eta_x(t)] - Q(\{x-1,x\})[\eta_x(t) - \eta_{x-1}(t)]}{1/N^2} \quad .$$

Rescaling time as $t/N^2 \to t$, in the limit $N \to \infty$ the particle density profile $\eta_x(t)/(1/N)$ tends to a function $u(z,t)$ solving the equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial z}\left(D \frac{\partial u}{\partial z}\right) \quad \text{(Fick)}.$$

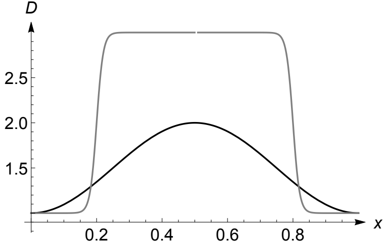
Recalling the diffusion coeffients

Consider

$$D_{\mathrm{c}}(x) = -\frac{1}{2}\cos(2\pi x) + \frac{3}{2}$$

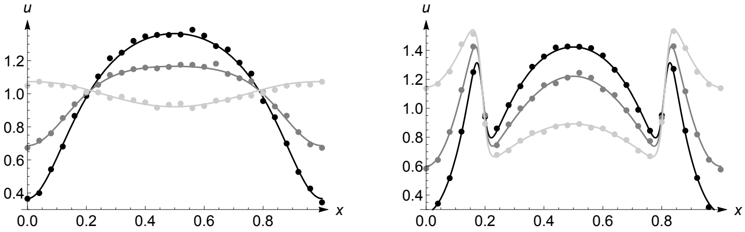
and

$$D_{\mathrm{d}}(z) = \begin{cases} 2 + \tanh(50(x - 0.2)) & x \le 0.5 \\ 2 - \tanh(50(x - 0.8)) & x > 0.5 \end{cases} .$$



Black curve for D_{c} and gray curve for D_{d} (mimics the discontinuous case).

The SIRW case



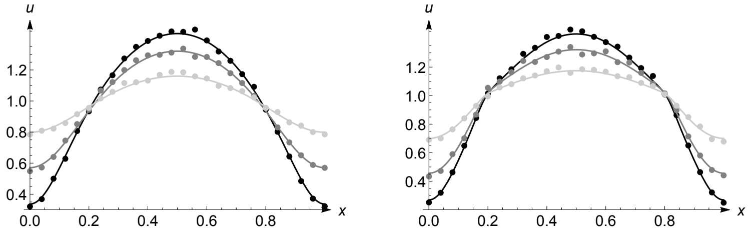
Particle profile of the Random Walk problem multiplied times N/M and solution of the Fokker–Planck problem with diffusion coefficient D_c on the left and D_d on the right.

Black, gray, and light gray curves and dots refer 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, $N = 101$ and $M = 10041$.

The EIRW case



Particle profile of the Random Walk problem multiplied times N/M and solution of the Fick problem with diffusion coefficient D_{c} on the left and D_{d} 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, $N = 101$ and $M = 10041$.

Comments

- the Fick and Fokker–Planck diffusion equations are possible macroscopic models for diffusion in presence of spatial inhomogeneities;
- we derive these two equations starting from stochastic microscopic particle models via the hydrodynamic limit;
- we associate the Fokker–Planck diffusione equation to local isotropy and the Fick equation to absence of local isotropy;
- if $\alpha(x) = D(z_x)$ and $Q(\{x, x+1\}) = G((z_x + z_{x+1})/2)$, for the stochastic general model we find the equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial z}\left(G \frac{\partial D u}{\partial z} \right).$$

Avanzo/Addenda

Focus on